DNA-like Structure of Surfaces

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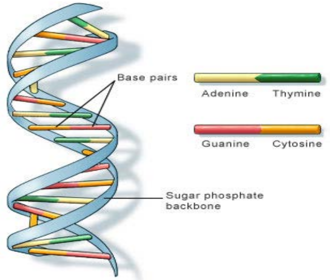
(in honor of the 75th birthday of Prof. Robert Plemmons)

Disclaimer

- This talk is about mathematics, not biology.
- This talk is elementary, involving only fundamental calculus.
- This work is just a beginning. More need be done.

- The importance of DNA is well documented.
  - Found in all living organisms.
  - Supplies the information for building all cell proteins.



- Basic structure of DNA:
  - Two strands coiled around to form a double helix.
  - Each rung of the spiral ladder consists of a pair of chemical groups called bases (of which there are four types)
  - Base pairing combines A to T and C to G, and the sequence on one strand is complementary to that on the other.
  - The specific sequence of bases constitutes the genetic information.

Take Home Message

- There is a considerably similar structure in all smooth functions.
- Will the structure determine the properties of the underlying function?
  - Sequencing: to interpret or to decode...
  - Synthesizing: to combine or to form...

Outline

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Gradient

- Given a scalar function

$$\eta : \mathbb{R}^n \longrightarrow \mathbb{R},$$

define the gradient of η by

$$\nabla\eta := \left[\frac{\partial\eta}{\partial x_1}, \ldots, \frac{\partial\eta}{\partial x_n}\right].$$

- Significance:
  - Points in the direction where the function $\eta(\mathbf{x})$ ascends most rapidly.
  - Attainable maximum rate of change is precisely $\|\nabla\eta(\mathbf{x})\|$.

Gradient Adaption

- Heat transfer by conduction.
  - Opposite to the temperature gradient and is perpendicular to the equal-temperature surfaces.
- Osmosis.
  - Passive transport of substances across the cell membrane down a concentration gradient without requiring energy use.
- Image gradients.
  - Fundamental building blocks in image processing such as edge detection and computer vision.

Jacobian

- Given a vector function

$$f : \mathbb{R}^n \longrightarrow \mathbb{R}^m,$$

define the Jacobian of f by

$$Jf := \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}.$$

  - A natural generalization of the gradient.
  - Both offer linear approximations.
  - Does not indicate critical directions or rates of change?

Singular Value Decomposition

- Any given matrix $A \in \mathbb{R}^{m \times n}$ enjoys a factorization of the form

$$A = V \Sigma U^\top.$$

  - Known as a singular value decomposition (SVD) of A.
- Singular vectors:
  - $V \in \mathbb{R}^{m \times m}$, $U \in \mathbb{R}^{n \times n}$ are orthogonal matrices.
- Singular values:
  - $\Sigma \in \mathbb{R}^{m \times n}$ is diagonal with nonnegative elements

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_\kappa > \sigma_{\kappa+1} = \ldots = 0.$$

  - $\kappa = \text{rank}(A)$.

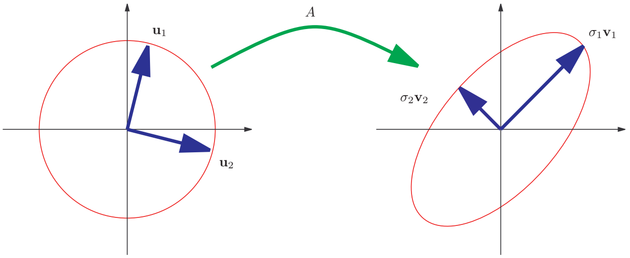
Variational Formulation

- Many ways to characterize the SVD of a matrix A.
- Cast as an optimization problem over the unit disk:

$$\max_{\|\mathbf{x}\|=1} \|A\mathbf{x}\|.$$

  - Unit stationary points $\mathbf{u}_i \in \mathbb{R}^n$ = Right singular vectors.
  - Singular values = $\|A\mathbf{u}_i\|$.

Geometric Meaning of SVD



- In the neighborhood of the origin:
  - Right singular vectors = Directions where the linear map A changes most critically.
  - Singular values = Extent of deformation.
- Similar role by the left singular vectors by the duality theory.

Linear Approximation

- Nearby any given point $\widetilde{\mathbf{x}}$, approximate $f(\mathbf{x})$ by the affine map

$$g(\mathbf{x}) := f(\widetilde{\mathbf{x}}) + f'(\widetilde{\mathbf{x}})(\mathbf{x} - \widetilde{\mathbf{x}}).$$

- Under the function g,
  - The unit sphere centered at $\widetilde{\mathbf{x}}$ gets mapped into an ellipsoid centered at $f(\widetilde{\mathbf{x}})$.
  - Semi-axes are aligned with the left singular vectors of $f'(\widetilde{\mathbf{x}})$.
  - Semi-axis lengths are precisely the singular values.

Infinitesimal Deformation

- Reducing the radius of the sphere,
  - Downsizes the ellipsoid proportionally.
  - Does not alter the directions of the semi-axes.
  - g becomes a more accurate approximation of f.
- The gradually reduced ellipsoids silhouette the images of the gradually reduced spheres under f.
- The SVD information of the linear operator $f'(\widetilde{\mathbf{x}})$ manifests the infinitesimal deformation property of the nonlinear map f at $\widetilde{\mathbf{x}}$.

Directional Derivatives

- Consider the norm of the directional derivative

$$\lim_{t \to 0} \left\| \frac{f(\widetilde{\mathbf{x}} + t\mathbf{u}) - f(\widetilde{\mathbf{x}})}{t} \right\| = \| f'(\widetilde{\mathbf{x}})\mathbf{u} \|.$$

  - **u** is an arbitrary unit vector.
- Along which direction will the norm of the directional derivative (Gâteaux derivative) be maximized?
  - The right singular vectors of $f'(\widetilde{\mathbf{x}})$!
- This is the generalization of the conventional gradient to vector functions.

Singular Vector Field

- At every point $\mathbf{x} \in \mathbb{R}^n$,
  - Have a set of orthonormal vectors pointing in particular directions related to the variation of f.
  - These orthonormal vectors form a natural frame point by point.
- Tracking down the “motion" of these frames might help to reveal some innate peculiarities of the underlying function f.

Dynamical Systems

- Let $(\sigma_i, \mathbf{u}_i, \mathbf{v}_i)$ = the ith singular triplet of $f'(\mathbf{x}_i)$. Interested in the solution flows:
  - $\mathbf{x}_i(t) \in \mathbb{R}^n$ defined by

$$\dot{\mathbf{x}}_i := \pm \mathbf{u}_i(\mathbf{x}_i), \quad \mathbf{x}_i(0) = \widetilde{\mathbf{x}}.$$

  - $\mathbf{y}_i(t) \in \mathbb{R}^m$ defined by

$$\dot{\mathbf{y}}_i := \pm \sigma_i(\mathbf{x}_i)\mathbf{v}_i(\mathbf{x}_i), \quad \mathbf{y}_i(0) = f(\widetilde{\mathbf{x}}).$$

- Minor notes:
  - Scaling ensures $\mathbf{y}_i(t) = f(\mathbf{x}_i(t))$.
  - Select the sign $\pm$ so as to avoid discontinuity jump.
  - Integrate in both forward and backward time.

Critical Points

- The vector field may not be well defined at certain points.
  - When singular values coalesce.
  - $f'(\mathbf{x})$ has multiple singular vector
  - Makes $\dot{\mathbf{x}}_i$ (or $\dot{\mathbf{y}}_i$) discontinuous.
- Not an issue of the factorization.
  - An analytic factorization as a whole for a function analytic in $\mathbf{x}$ does exist.
  - The continuity of a fixed order singular vectors, say, $\mathbf{u}_1(\mathbf{x})$, may not be maintained.

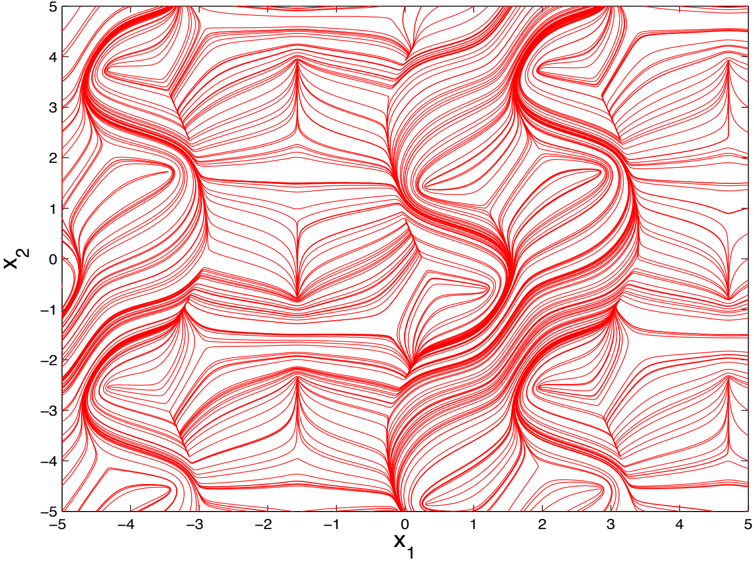
First Singular Curve

- Moves in the direction along which $f(\mathbf{x})$ changes most rapidly, when measured in the Euclidean norm.
- Serves as the backbone in the moving frame.
- Can be demonstrated and explained in the case $f : \mathbb{R}^2 \rightarrow \mathbb{R}^n$.
  - Parametric surfaces.
- More need be done in higher dimensional spaces.

Example 1

$$\begin{bmatrix} \sin(x_1 + x_2) + \cos(x_2) - 1 \\ \cos(2\,x_1) + \sin(x_2) - 1 \end{bmatrix}$$

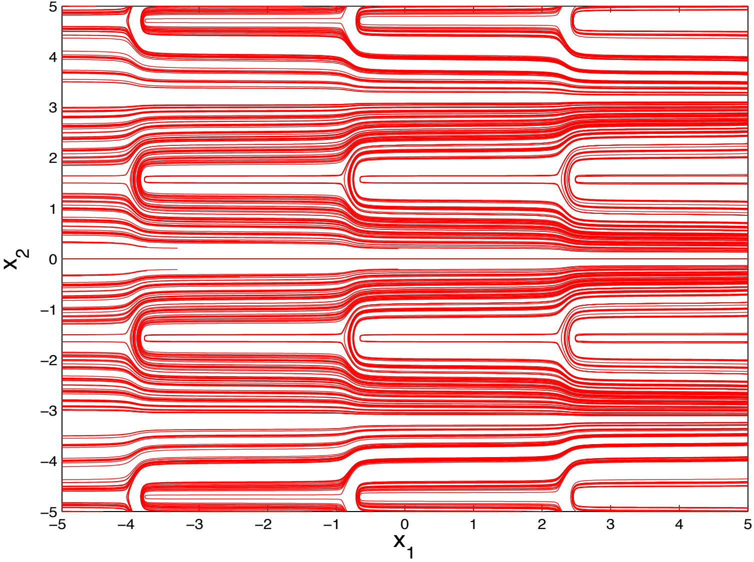
Right Singular Curves for Example 1



Example 2a

$$\begin{bmatrix} e^{x_1}\cos(x_2) \\ 20e^{x_1}\sin(x_1) \end{bmatrix}$$

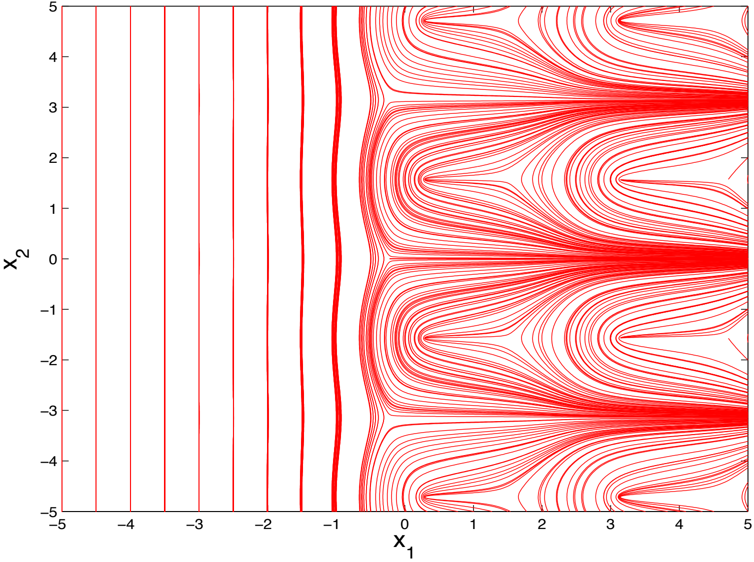
Right Singular Curves for Example 2a



Example 2b

$$\begin{bmatrix} e^{x_1}\cos(x_2) \\ e^{x_1}\sin(x_1) \\ x_2 \end{bmatrix}$$

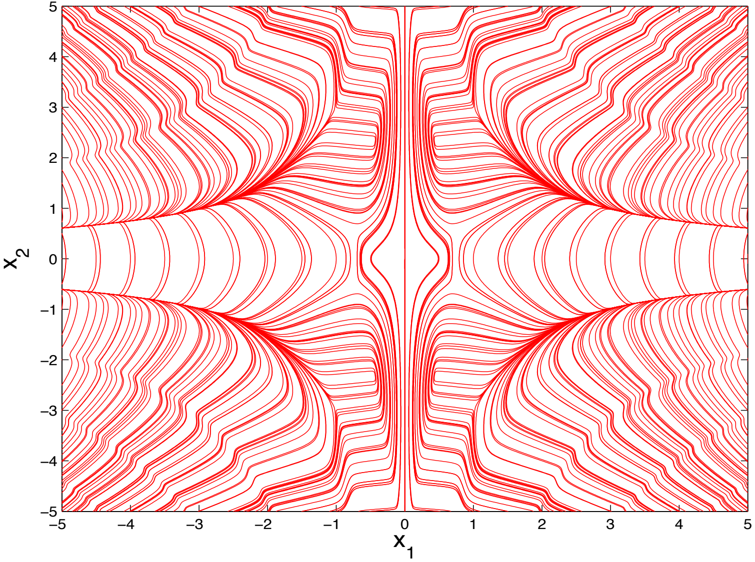
Right Singular Curves for Example 2b



Example 3

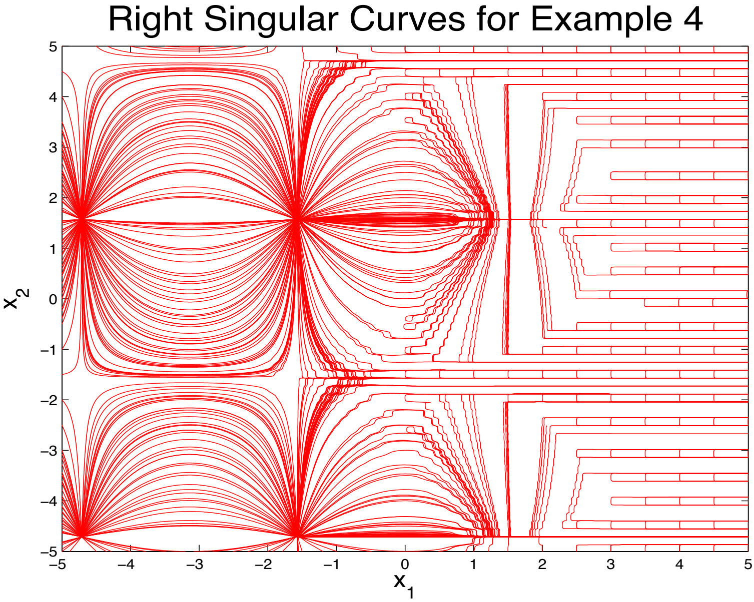
$$\begin{bmatrix} 4 + x_1 \cos(x_2/2) \\ x_2 \\ x_1 \sin(x_1 x_2/2) \end{bmatrix}$$

Right Singular Curves for Example 3



Example 4

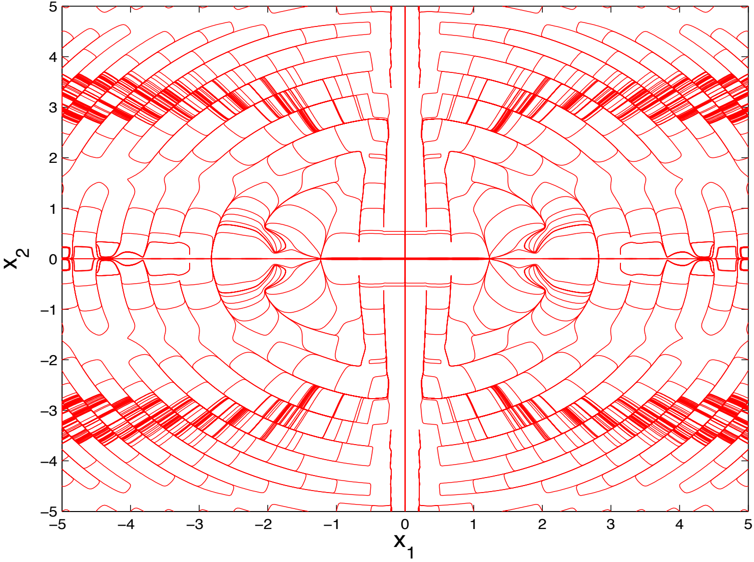
$$\begin{bmatrix} e^{x_1} \cos(20x_2) \\ 20e^{sin(x_2)} \sin(x_1) \end{bmatrix}$$


Right Singular Curves for Example 4
5
4
3
2
1
0
−1
−2
−3
−4
−5
x2
−5
−4
−3
−2
−1
0
1
2
3
4
5
x1

Example 5

$$\begin{bmatrix} \sin(x_1^2 + x_2^2)\cos(x_2) \\ 2e^{-2x_2^2 x_1^2}\cos(10\sin(x_1)) \end{bmatrix}$$

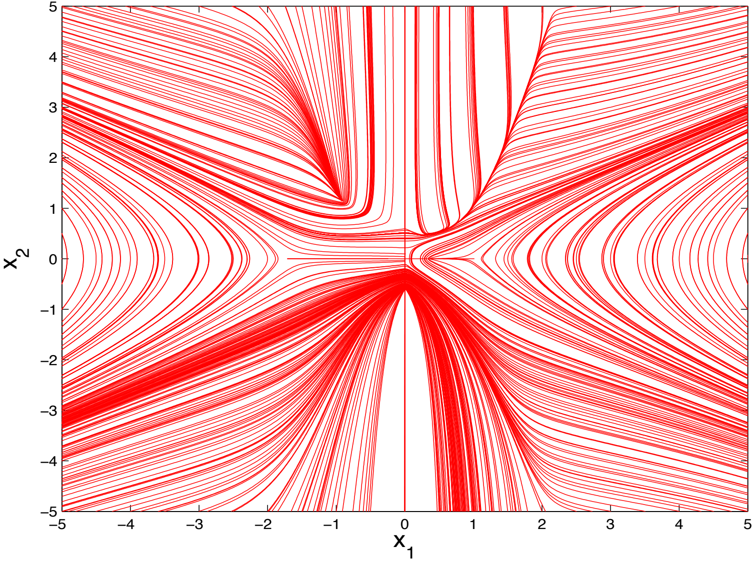
Right Singular Curves for Example 5



Example 7

$$\begin{bmatrix} x_1 - \frac{x_1^2}{3} + x_1 x_2^2 \\ x_2 - \frac{x_2^3}{6} + x_2 x_1^3 \\ x_1^2 - x_2^3 \end{bmatrix}$$

Right Singular Curves for Example 7

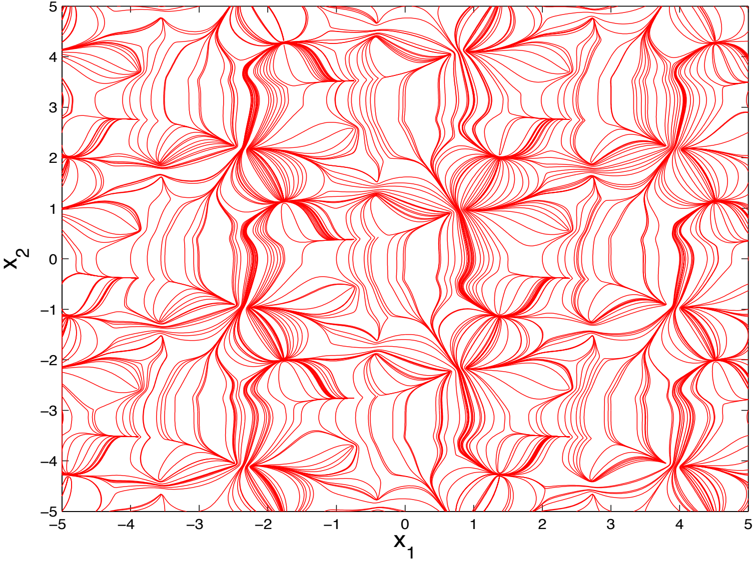


Example 8

$$\begin{bmatrix} \frac{1}{2}\left(2\rho^2 - \phi^2 - \psi^2 + 2\phi\psi(\phi^2 - \psi^2) + \psi\rho(\rho^2 - \psi^2) + \rho\phi(\phi^2 - \rho^2)\right) \\ \frac{\sqrt{3}}{2}\left(\phi^2 - \psi^2 + (\psi\rho(\psi^2 - \rho^2) + \rho\phi(\phi^2 - \rho^2))\right) \\ (\rho + \phi + \psi)\left((\rho + \phi + \psi)^3 + 4(\phi - \rho)(\psi - \phi)(\rho - \psi)\right) \end{bmatrix}$$

$$\text{with} \begin{cases} \rho = \cos(x_1)\sin(x_2) \\ \phi = \sin(x_1)\sin(x_2) \\ \psi = \cos(x_2) \end{cases}$$

Right Singular Curves for Example 8



Why?

A Closer Look

- Write

$$f'(\mathbf{x}) = \left[\ \mathbf{a}_1(\mathbf{x}), \mathbf{a}_2(\mathbf{x})\ \right].$$

- Define scalar functions

$$\begin{cases} n(\mathbf{x}) & := & \|\mathbf{a}_2(\mathbf{x})\|^2 - \|\mathbf{a}_1(\mathbf{x})\|^2, \\ o(\mathbf{x}) & := & 2\mathbf{a}_1(\mathbf{x})^\top \mathbf{a}_2(\mathbf{x}). \end{cases}$$

  - $n(\mathbf{x})$ measures the disparity of lengths.
  - $o(\mathbf{x})$ measures nearness of orthogonality.

Critical Curves

- Define

$$\begin{cases} \mathcal{N} := \{\mathbf{x} \in \mathbb{R}^n \mid n(\mathbf{x}) = 0\}\,, \\ \mathcal{O} := \{\mathbf{x} \in \mathbb{R}^n \mid o(\mathbf{x}) = 0\}\,. \end{cases}$$

- Each forms generically a 1-dimensional manifold in $\mathbb{R}^2$.
  - Possibly composed of multiple curves or loops.
  - Will play the role of “polynucleotide" connecting a string of interesting points.

First Right Singular Pair

- The first singular value of $f'(\mathbf{x})$:

$$\sigma_1(\mathbf{x}) := \left(\frac{1}{2}\left(\|\mathbf{a}_1(\mathbf{x})\|^2 + \|\mathbf{a}_2(\mathbf{x})\|^2 + \sqrt{o(\mathbf{x})^2 + n(\mathbf{x})^2}\right)\right)^{1/2}$$

- The first right singular vector:

$$\mathbf{u}_1(\mathbf{x}) := \frac{\pm 1}{\sqrt{1+\omega(\mathbf{x})^2}} \begin{bmatrix} \omega(\mathbf{x}) \\ 1 \end{bmatrix}.$$

with

$$\omega(\mathbf{x}) := \begin{cases} \frac{o(\mathbf{x})}{n(\mathbf{x})+\sqrt{o(\mathbf{x})^2+n(\mathbf{x})^2}}, & \text{if } n(\mathbf{x}) > 0, \\ \frac{-n(\mathbf{x})+\sqrt{o(\mathbf{x})^2+n(\mathbf{x})^2}}{o(\mathbf{x})}, & \text{if } n(\mathbf{x}) < 0. \end{cases}$$

  - Take the limit if $\omega(\mathbf{x})$ becomes infinity.

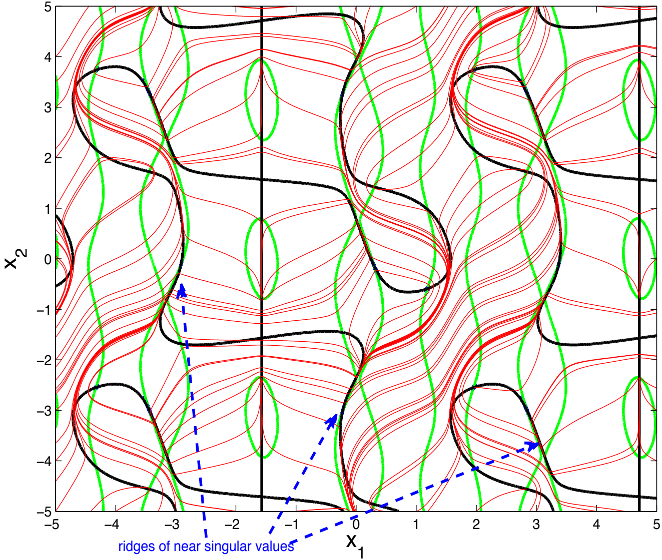
Crossings

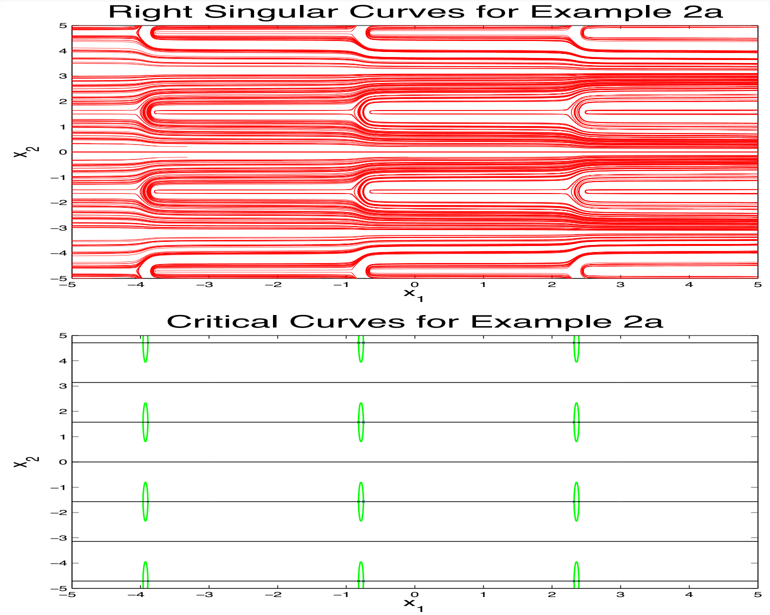
- When singular curves coming across critical curves, their tangent vectors point in specific directions.
- Orientations of tangent vectors:
  - At $\mathcal{N} - \mathcal{O}$, are parallel to either $[1,\ 1]^\top$ or $[1,\ -1]^\top$, depending on whether $o(\mathbf{x})$ is positive or negative.
  - At $\mathcal{O} - \mathcal{N}$, are parallel to $[0,\ 1]^\top$ or $[1,\ 0]^\top$, depending on whether $n(\mathbf{x})$ is positive or negative.

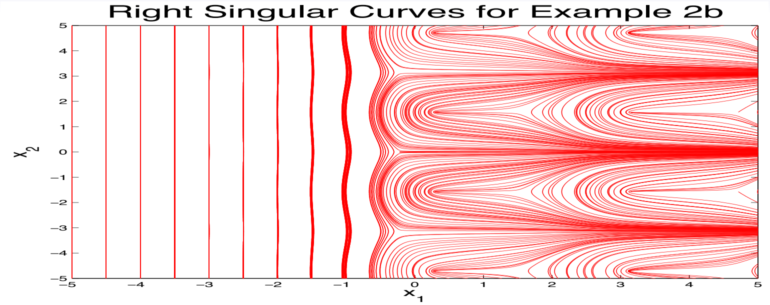
Singular Points

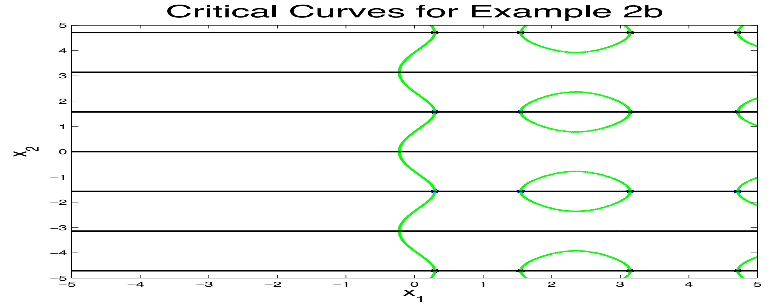
- $\mathcal{N} \bigcap \mathcal{O}$ = *singular points*.
- At singular points,
  - Singular values coalesce.
  - The (right) singular vectors become ambiguous.
  - Singular curves are“terminated" or “reborn".
- The angles cut by $\mathcal{N}$ and $\mathcal{O}$ at the singular point affects the intriguing dynamics observed.
  - The 1-dimensional manifolds $\mathcal{N}$ and $\mathcal{O}$ string singular points together along their strands.

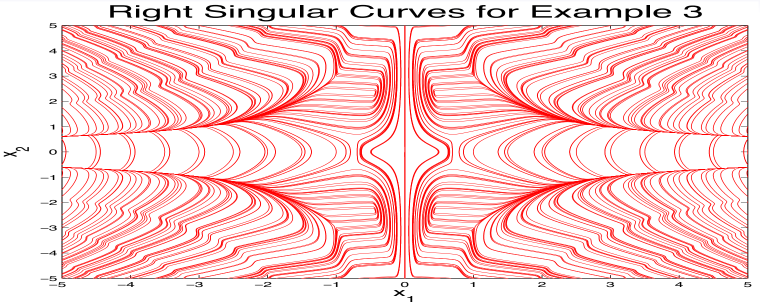
Critical Curves and Singular Curves for Example 1

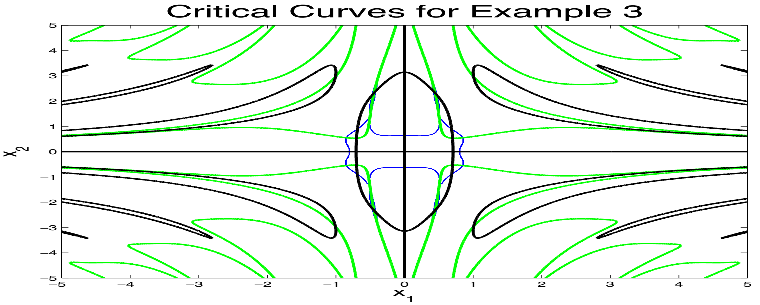



Right Singular Curves for Example 2a
x2
x1
Critical Curves for Example 2a
x2
x1

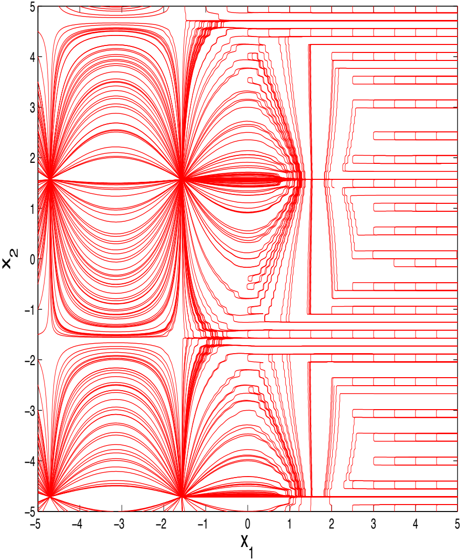

Right Singular Curves for Example 2b
x_2
x_1
5
4
3
2
1
0
−1
−2
−3
−4
−5


Critical Curves for Example 2b
x_2
x_1
5
4
3
2
1
0
−1
−2
−3
−4
−5

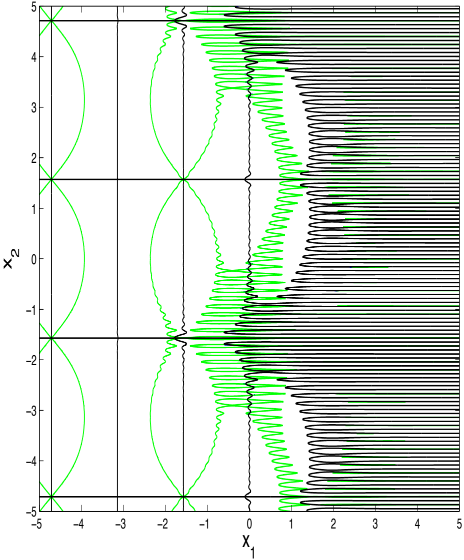

Right Singular Curves for Example 3
x2
x1
5
4
3
2
1
0
−1
−2
−3
−4
−5


Critical Curves for Example 3
x2
x1
5
4
3
2
1
0
−1
−2
−3
−4
−5

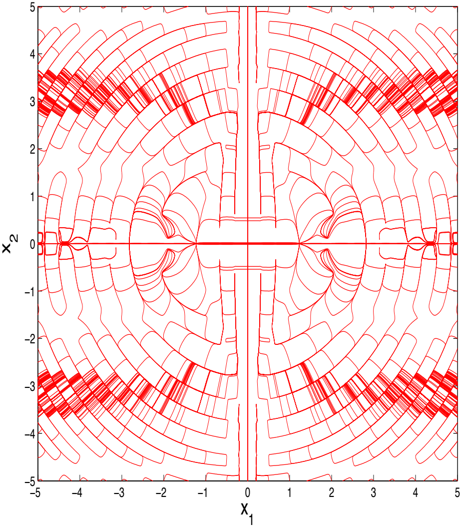
Right Singular Curves for Example 4



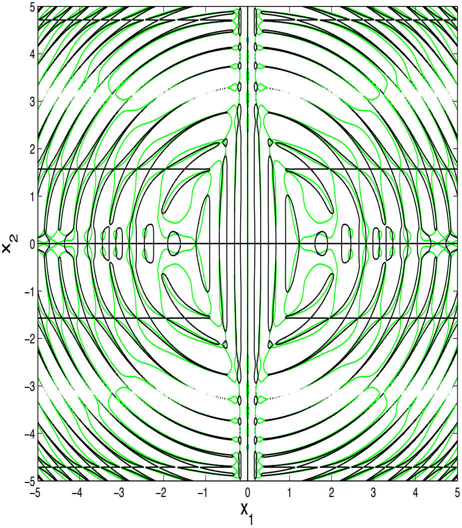
Critical Curves for Example 4

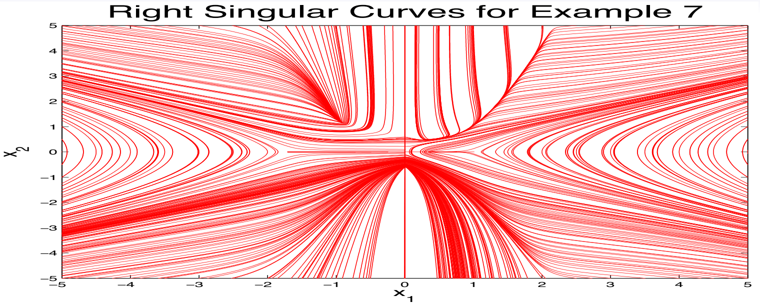


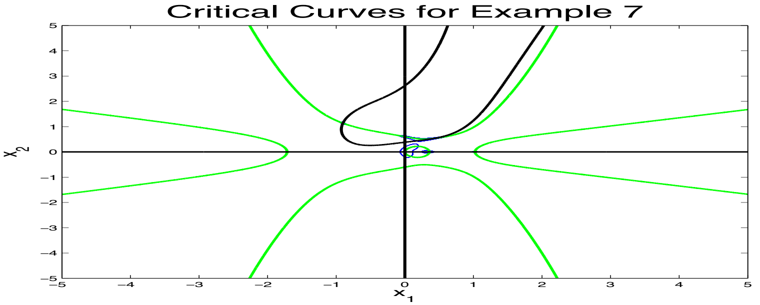
Right Singular Curves for Example 5

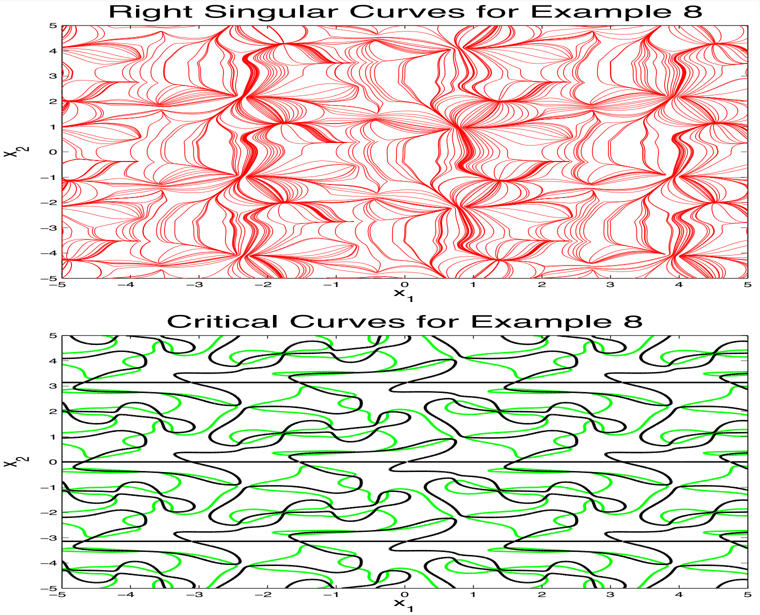


Critical Curves for Example 5




Right Singular Curves for Example 7
x_2
x_1
5
4
3
2
1
0
−1
−2
−3
−4
−5
−5
−4
−3
−2
−1
0
1
2
3
4
5

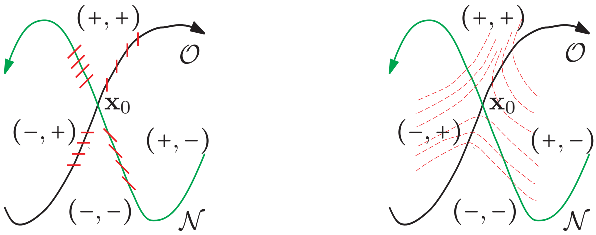

Critical Curves for Example 7
x_2
x_1
5
4
3
2
1
0
−1
−2
−3
−4
−5
−5
−4
−3
−2
−1
0
1
2
3
4
5


Right Singular Curves for Example 8
x2
x1
Critical Curves for Example 8
x2
x1

Curvilinear Coordinate System

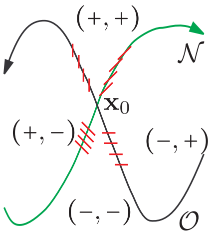
- Denote the α-*halves* portions of $\mathcal{N}$ and $\mathcal{O}$ by by n_α and o_α, where
  - The crossing singular vectors are parallel to the unit vectors $\mathbf{u}_{n_\alpha} := \frac{1}{\sqrt{2}}[1,1]^\top$ and $\mathbf{u}_{o_\alpha} := [0,1]^\top$.
- Flag the sides of n_α and o_α by arrows .
  - Naturally divides the neighborhood of $\mathbf{x}_0$ into “quadrants" distinguished by the signs $(\mathrm{sgn}(n(\mathbf{x})), \mathrm{sgn}(o(\mathbf{x})))$.
- When the “orientation" is changed, the nearby dynamical behavior might also change its topology.

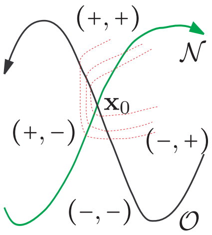
A Scenario of Propellant



- Red segments = tangent vectors crossing the critical curves.
  - Take into account the signs of $o(\mathbf{x})$ and $n(\mathbf{x})$.
- Invariant on each half of the critical curves.
- Flows of singular curves near $\mathbf{x}_0$ should move away from $\mathbf{x}_0$ as a repellant.

A Scenario of Roundabout

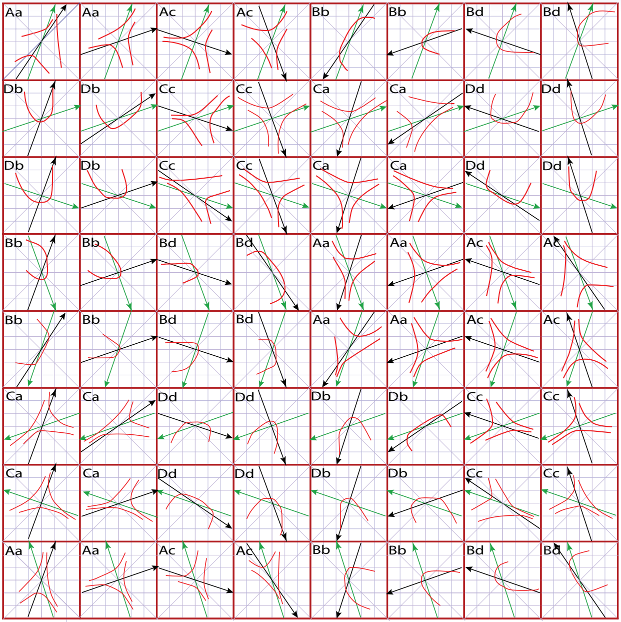




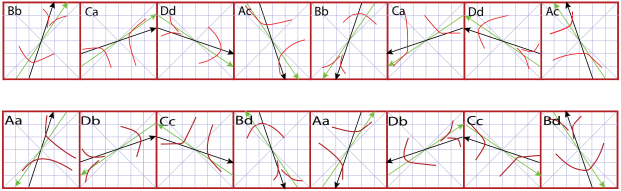
Generic Behaviors

- Divide the plane into eight sectors with a central angle $\frac{\pi}{4}$.
- Relative position of n_α and o_α with respect to these sectors is critical for deciding the local behavior.

Regular Cases



Mutative Cases



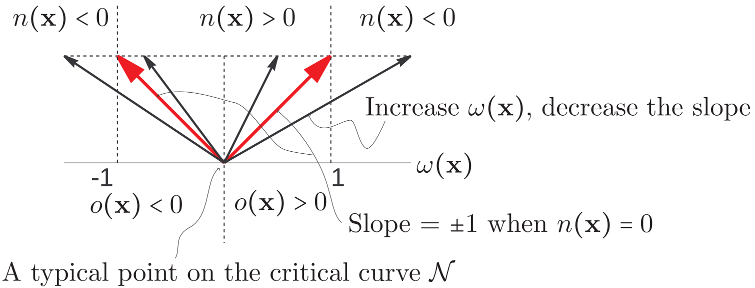
Second Derivative

- Express $\omega(\mathbf{x})$ as

$$\omega(\mathbf{x}) := \begin{cases} \operatorname{sgn}(o(\mathbf{x})) - \frac{n(\mathbf{x})}{o(\mathbf{x})} + \frac{\operatorname{sgn}(o(\mathbf{x}))n(\mathbf{x})^2}{2o(\mathbf{x})^2} + O\left(n(\mathbf{x})^3\right), & \text{near } n(\mathbf{x}) = 0, \\ \frac{o(\mathbf{x})}{2n(\mathbf{x})} - \frac{o(\mathbf{x})^3}{8n(\mathbf{x})^3} + \frac{o(\mathbf{x})^5}{16n(\mathbf{x})^5} + O\left(o(\mathbf{x})^7\right), & \text{near } o(\mathbf{x}) = 0 \text{ and if } n(\mathbf{x}) > 0, \\ \frac{-1}{\frac{o(\mathbf{x})}{2n(\mathbf{x})} - \frac{o(\mathbf{x})^3}{8n(\mathbf{x})^3} + \frac{o(\mathbf{x})^5}{16n(\mathbf{x})^5} + O\left(o(\mathbf{x})^7\right)}, & \text{near } o(\mathbf{x}) = 0 \text{ and if } n(\mathbf{x}) < 0. \end{cases}$$

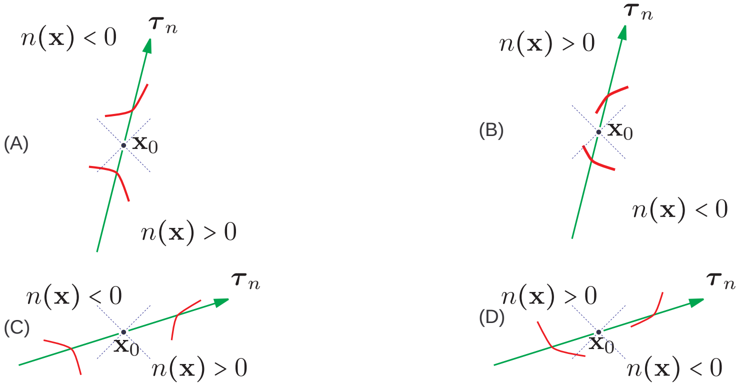
  - The first derivative of $\mathbf{x}_1(t)$ is related to $\omega(\mathbf{x}_1(t))$.
    - The first term of $\omega(\mathbf{x})$ estimates the the second derivative of $\mathbf{x}_1(t)$.
  - Can characterize the concavity property observed.

Variation near $\mathcal{N}$

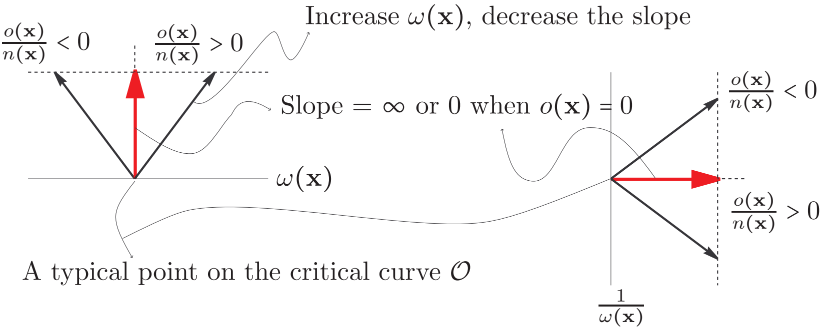


- In the direction $\mathbf{u}_{n_\alpha}$, $\omega(\mathbf{x}(t))$ must be increased if $\mathbf{x}(t)$ moves to the side where $n(\mathbf{x}) < 0$.
  - The slope of $\mathbf{u}_1(\mathbf{x}(t))$ must be less than 1.
- Only four basic ways to cross $\mathcal{N}$.

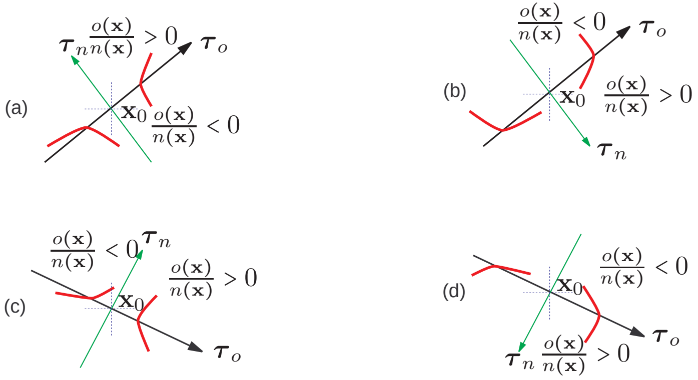
Four Bases along $\mathcal{N}$



Variation near $\mathcal{O}$



Four Bases along $\mathcal{O}$



Pairing

- Entire dynamics can be classified into 8 categories.
  - These base parings are Aa, Ac, Bb, Bd, Ca, Cc, Db, and Dd only, with no other possible combinations.
- Each base pairing results in 8 dynamics in the regular cases and 2 in the mutative cases.
  - Distinctive by their characteristic traits.
  - Fascinating, but no time in this talk.
- Identify each dynamics by two letters of base paring at the upper left corner.

Allowable Pairings with Two Polynucleotides

	A	B	C	D
a	[Aa]	Ba	[Ca]	Da
b	Ab	[Bb]	Cb	[Db]
c	[Ac]	Bc	[Cc]	Dc
d	Ad	[Bd]	Cd	[Dd]

- What happens to other pairings?

Trait Characterization

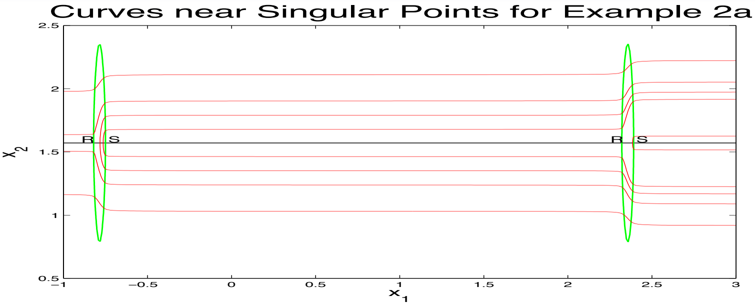
- Base pairings characterize dynamical details.
- Can also characterize the general behavior by a single quantity.
  - Define $\theta(n_\alpha, o_\alpha)$ = Angles measured clockwise from $\boldsymbol{\tau}_n$ and to $\boldsymbol{\tau}_o$.
  - Assume the generic condition that $\boldsymbol{\tau}_n$ is not forming an angle $\frac{\pi}{4}$ with the north.
  - Singular point $\mathbf{x}_0$ is
    - A repeller, if $0 < \theta(n_\alpha, o_\alpha) < \pi$.
    - A roundabout, if $\theta(n_\alpha, o_\alpha) > \pi$.
- Crossovers/hybrids are possible.
- $\vdots$
- Too detailed to include here.

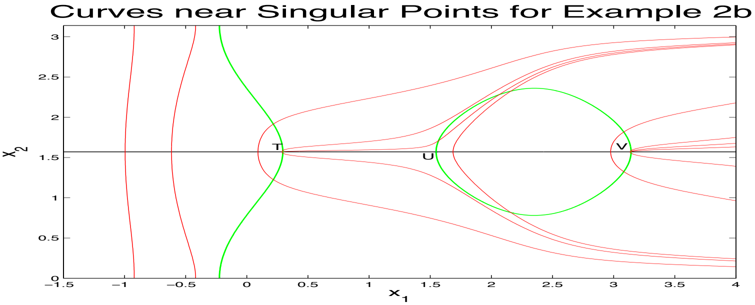
Making Mosaics

- Classify of all possible local behaviors.
  - A simplistic collection of “tiles" for the delicate and complex “mosaics".
- Arrange pieces of mosaics along the strands of $\mathcal{N}$ and $\mathcal{O}$
  - Inherent characteristics of the local dynamics form the various patterns and variations of the underlying function.

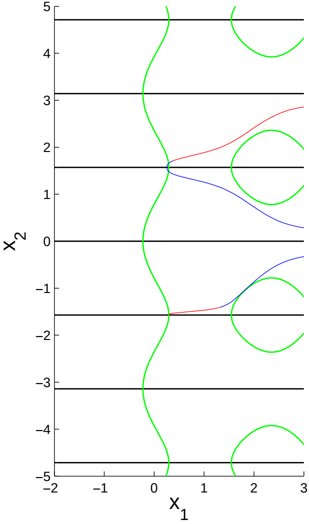
A Comparison

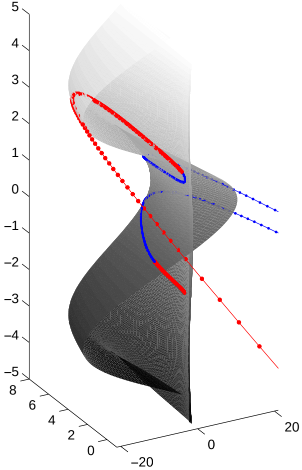
- Consider examples 2a and 2b.
  - Easy critical curves.
    - $\mathcal{O}$ forms horizontal lines with alternating $o(\mathbf{x})$ in between.
    - $\mathcal{N}$ forms closed loops.
    - One additional vertical, continuous, ogee $\mathcal{N}$ curve in Example 2b.
    - $n(\mathbf{x}) > 0$ inside the loops and to the left of the ogee curve.
- Similar, but different dynamics.


Curves near Singular Points for Example 2a
R
S
R
S
x_2
x_1
2.5
2
1.5
1
0.5
−1
−0.5
0
0.5
1
1.5
2
2.5
3

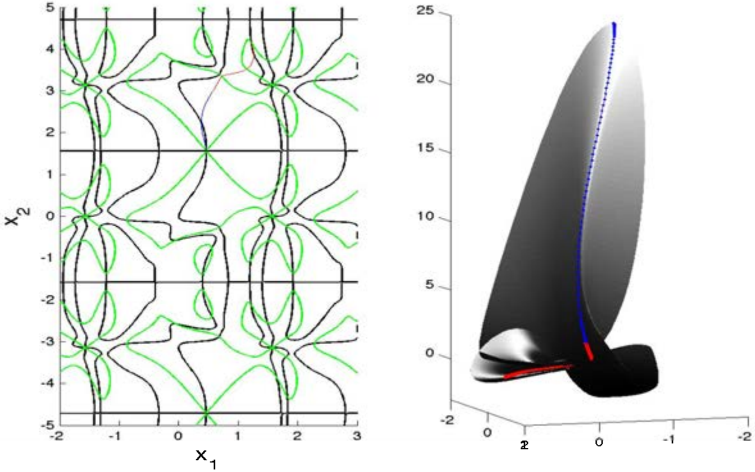

Curves near Singular Points for Example 2b
T
U
V
x_2
x_1
3
2.5
2
1.5
1
0.5
0
−1.5
−1
−0.5
0
0.5
1
1.5
2
2.5
3
3.5
4

Left Singular Curves

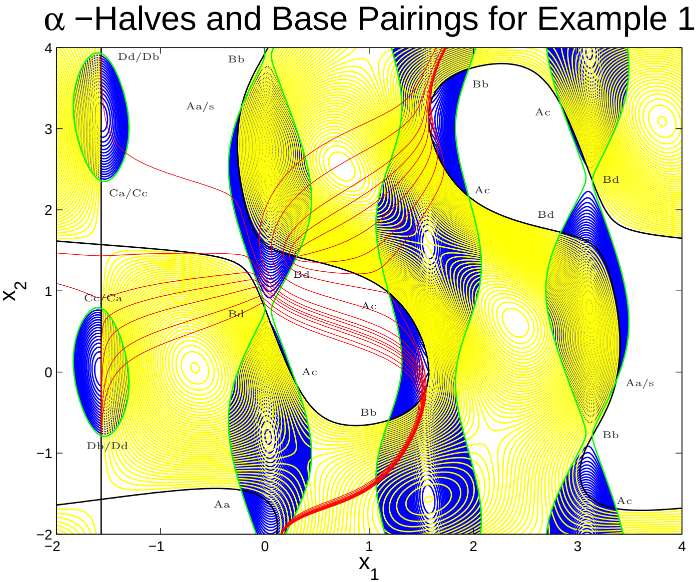




Boy's Face



A Jigsaw Puzzle



Conclusion

- Gradient adaption is an important mechanism in nature.
  - Generalization to the Jacobian does not “discriminate" directions per se.
- Adaption information is coded in the singular curves.
  - Form a natural moving frame telling intrinsic properties per the given function.
  - Result in intricate and complicated patterns.
- Global behavior in general and interpretation in specific are not conclusively understood yet.
  - Two stands joined by singular points with one of eight distinct base pairings make up the underlying function.
  - Amazingly analogous to the DNA structure essential for all known forms of life.
- Are the patterns discovered “the trace of DNA" within an abstract, “inorganic" function?