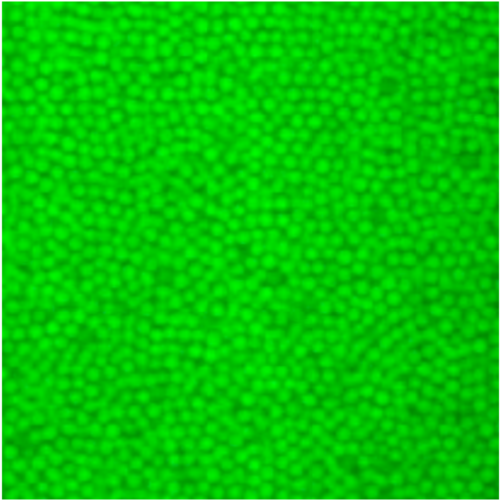
3. What do extremal trajectories look like?

a glass



Density functional theory

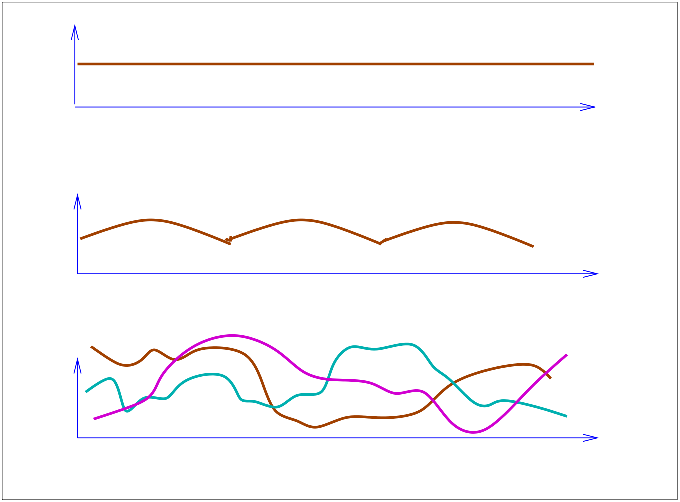
a mean-field free energy

$$\boxed{F[\rho] = T \int d^3\mathbf{x}\ \rho[\ln \rho(\mathbf{x}) - 1] - \frac{1}{2} \int d^3\mathbf{x}\ d^3\mathbf{x}'\ [\rho(\mathbf{x}) - \rho_o] C(\mathbf{x} - \mathbf{x}') [\rho(\mathbf{x}') - \rho_o]}$$

has many local minima, solutions of

$$\frac{\delta F[\rho(\mathbf{x})]}{\delta \rho} = 0$$

liquid – crystal + many amorphous



Analogy with dynamic systems

Ruelle + Aubry-Mather theory

space	$\rightarrow$	time

$\rho(x) = \rho_o$ liquid	$\rightarrow$	fixed point
crystal	$\rightarrow$	periodic solution
amorphous	$\rightarrow$	chaotic solution

Density functional theory reduced to the essential

$$F[\rho(\mathbf{x})] = \int d^3\mathbf{x}\ \rho[\ln\rho(\mathbf{x}) - 1] - \frac{1}{2}\int d^3\mathbf{x}\ d^3\mathbf{x}'\ [\rho(\mathbf{x}) - \rho_o]C(\mathbf{x} - \mathbf{x}')[\rho(\mathbf{x}') - \rho_o]$$

$$\downarrow$$

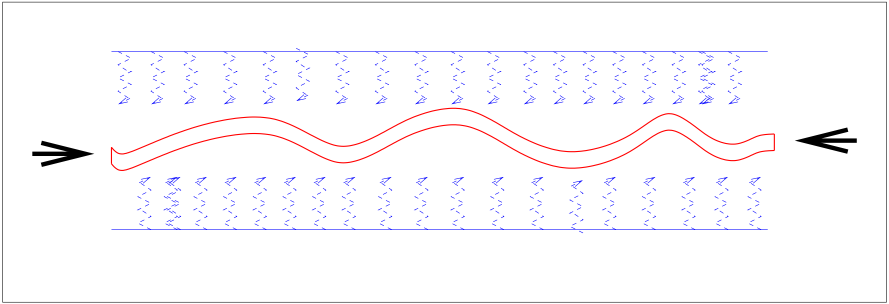
$$F[\rho(\mathbf{x})] = \int d^3\mathbf{x}\ V(\rho) - \frac{1}{2}\int d^3\mathbf{x}\ \ (a_o\rho^2 - a_1(\nabla\rho)^2 + a_2(\nabla^2\rho)^2 + ...)$$

Swift-Hohenberg like

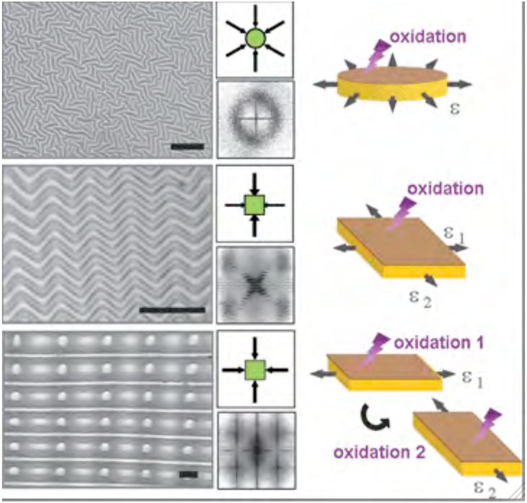
What are then the stationary solutions of

$$F[\rho(\mathbf{x})] = \int d^3\mathbf{x}\, V(\rho) - \frac{1}{2}\int d^3\mathbf{x}\ \ (a_o\rho^2 - a_1(\nabla\rho)^2 + a_2(\nabla^2\rho)^2)$$

and , in particular, its ground state?



constrained, elastic


oxidation
ε
oxidation
ε_1
ε_2
oxidation 1
ε_1
oxidation 2
ε_2

Chiche, et al

One dimension

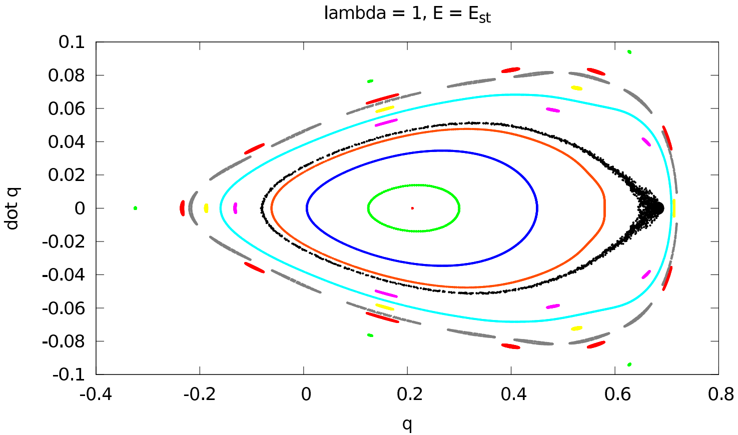
$$F[\rho(\mathbf{t})] = \int dt\, V(\rho) - \frac{1}{2}\int dt\ \ (a_o\rho^2 - a_1(\dot{\rho})^2 + a_2(\ddot{\rho})^2)$$

the action corresponding, in the coordinates $(\rho, \hat{\rho})$ and $(w, \hat{w})$ to

$$\mathcal{H} = V(\rho) + \tfrac{1}{2}a_o\rho^2 - \tfrac{1}{2}a_1 w^2 + w\hat{\rho} - \tfrac{1}{2}\hat{w}^2$$

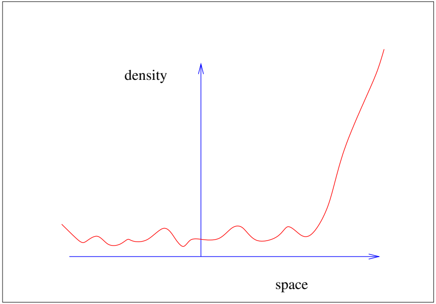
a non-linear, unbounded, Hamiltonian with more than one degree of freedom

and now we really have chaos in the sense of dynamical systems



$\rho(x)$ **versus** $\frac{d\rho}{dx}$

we search for bounded solutions with small free energies



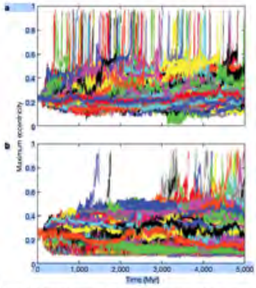


Figure 1 | Mercury's eccentricity over 5 Gyr. Evolution of the maximum

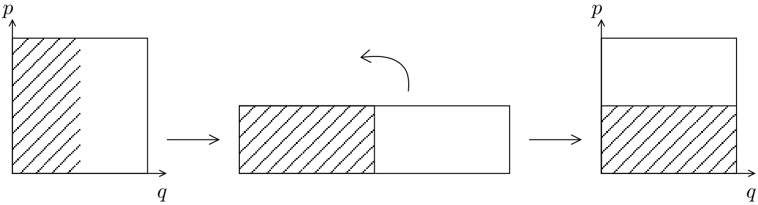
and we unexpectedly find ourselves back with a planetary stability -like problem!

Density functional theory in higher dimension:

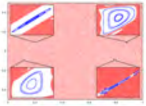
Chaos with several variables *and* **three dimensional time...**

What do extremal trajectories look like?

The baker's map

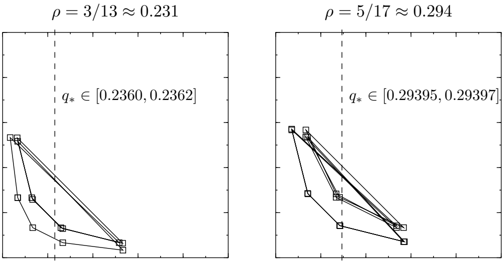


... is as chaotic as you can be.



And yet, orbits minimising a function, e.g.

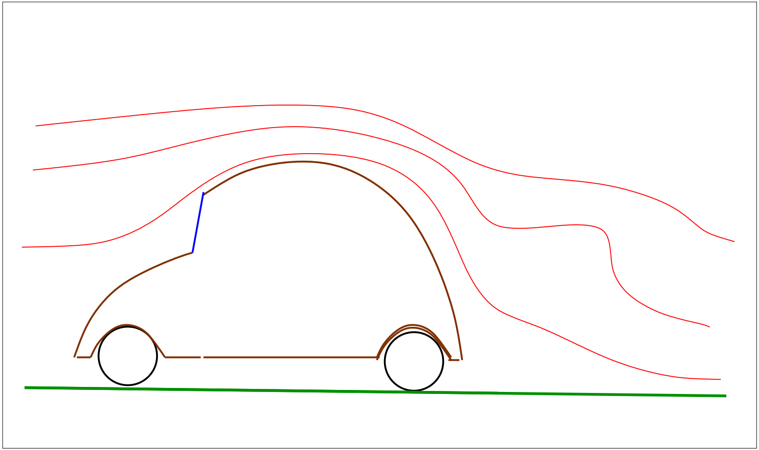
$$\mathcal{A} \equiv \int dt\, (q(t) - q_*)^2$$



are periodic or quasiperiodic but unstable!

Hunt and Ott — Khan-Dang Nguyen Thu Lam, JK , D Levine

If this metaphor is good, we should see:



during exceptional times

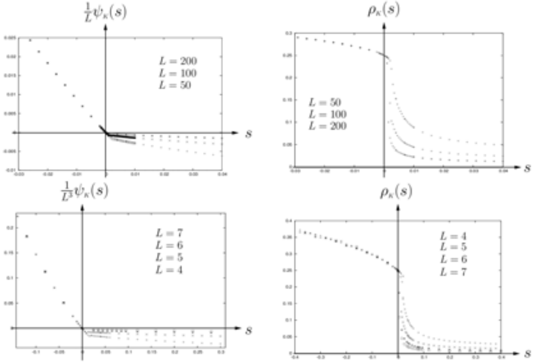
- **large deviations are sometimes important. we know how to simulate them efficiently**
- **extreme events in chaotic systems may be expected to be ordered, but unstable**
- **deep glassy states are analogous to extreme trajectories of chaotic systems with space $\leftrightarrow$ time**

4. Large deviations and Metastability

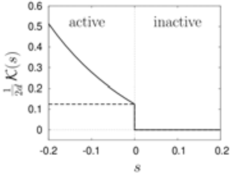
Dynamical phase transitions

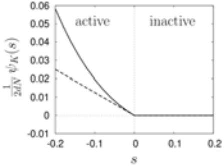
large deviations of the activity

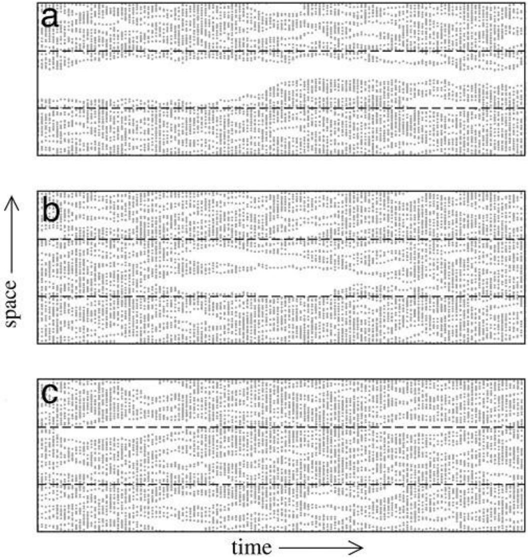
JP Garrahan, RL Jack, V Lecomte, E Pitard, K van Duijvendijk, and Frederic van Wijland



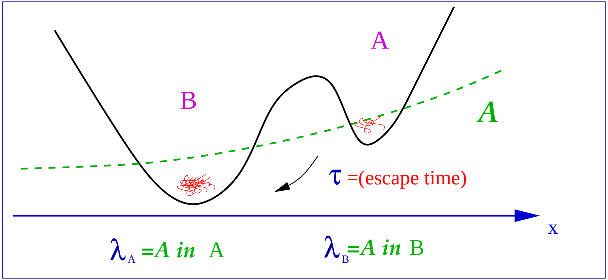

T
Active
Inactive
Criticality
s


$\frac{1}{2d}\mathcal{K}(s)$
0.6
0.5
0.4
0.3
0.2
0.1
0
active
inactive
-0.2
-0.1
0
0.1
0.2
s


$\frac{1}{2dN}\psi_K(s)$
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
active
inactive
-0.2
-0.1
0
0.1
0.2
s


a
b
c
space
time

Competition between colonies



$$\lambda_A - \lambda_B + 1/\tau$$

- A collection of metastable states

- **each with its own emigration rate**

- **and its cloning/death rates dependent upon the observable**

One way to understand the relation between metastability and large deviations

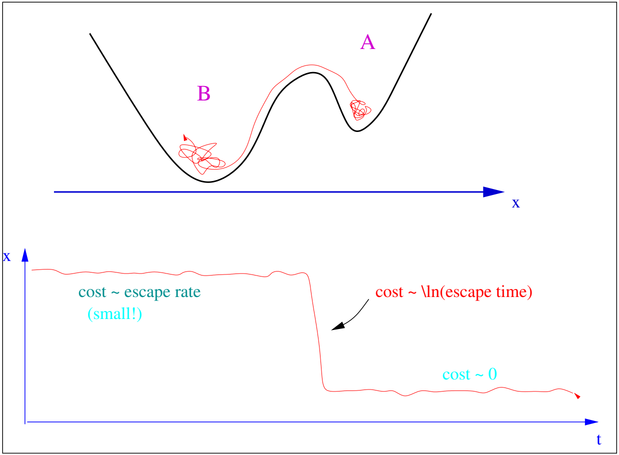
Large deviations with metastability as first order transitions: space time view

A dynamics: e.g. Langevin: $\dot{x}_i = -f_i(x) + \eta_i$

= add all trajectories with weight: $S[x] = -\frac{1}{T}\int dt\ \{\dot{x}_i + f_i(x)\}^2 ...$

For small T, all trajectories that stay in a metastable state $\dot{x}_i = f_i = 0$ contribute 'almost' the same

in detail



ice-water at -0.001 ^oC

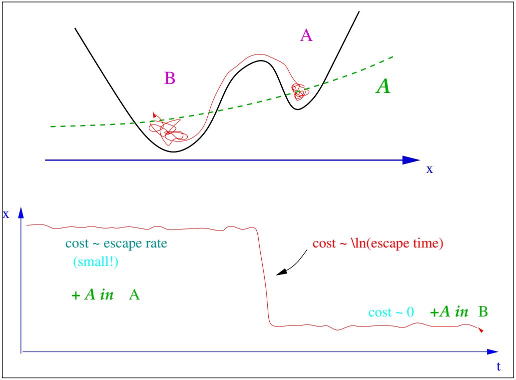
Large deviations and first order

Large deviation function $\langle e^{\lambda \int dt A[x]} \rangle = \int d\lambda P(A) e^{-\lambda A}$

= trajectories with weight:

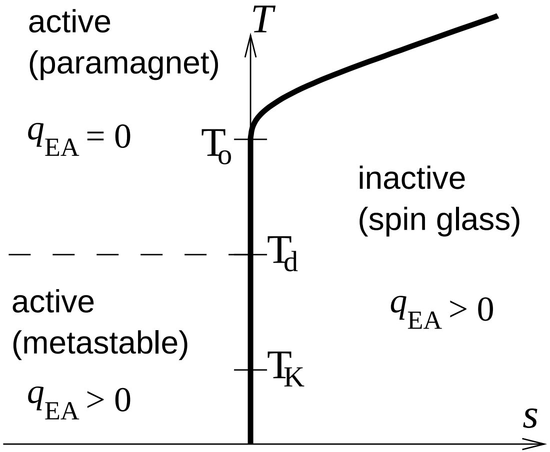
$$S_A[x] = \frac{1}{T} \int dt \; \{\dot{x}_i + f_i(x)\}^2 ... + \lambda A(x)$$

The observable A chooses the phase, for λ just larger than the escape rate

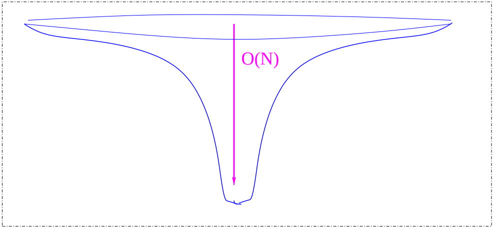


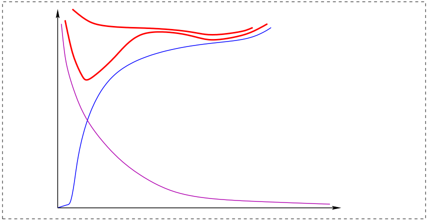
Another way to understand the relation between metastability and large deviations

Activity, ‘glass’ transition Garrahan and Jack



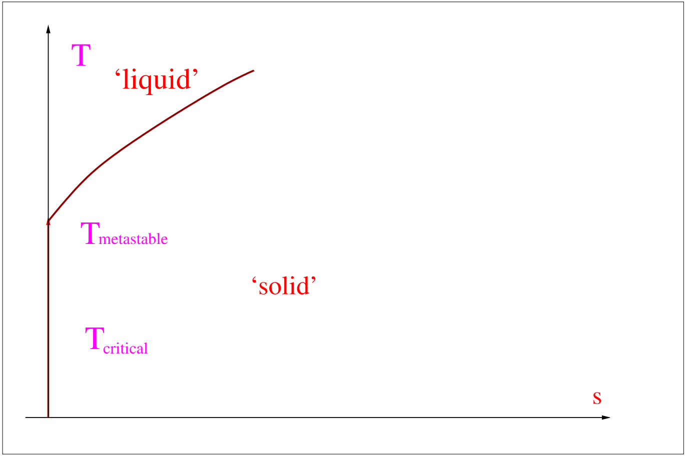
Champagne cup potential - spherical coordinates





A Langevin process for the radius: $\dot{r} = -\frac{d}{dr}\left\{V - (N-1)T\ln r\right\}$

Champagne cup potential - Phase diagram



5. Cell dynamics with selection

- **A cell performs complex dynamics: DNA codes for the production of proteins, which themselves modify how the reading is done. A bit like a program and its RAM content.**
- **DNA contains about the same amount of information as the TeXShop program for Mac**
- **This dynamics admits more than one attractor: same DNA yields liver and eye cells...**
- **The dynamical state is inherited.**
- **On top of this process, there is the selection associated to the death and reproduction of individual cells**

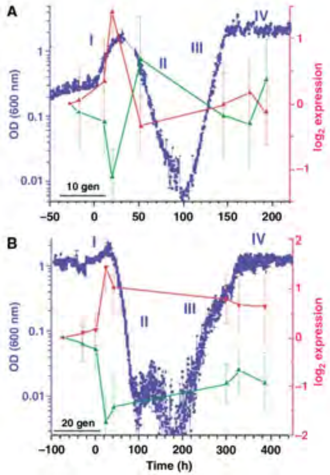
Stern, Dror, Stolovicki, Brenner, and Braun

An arbitrary and dramatic rewiring of the genome of a yeast cell:

the presence of glucose causes repression of histidine biosynthesis, an essential process

Cells are brutally challenged in the presence of glucose, nothing in evolution prepared them for that!

Stern, Dror, Stolovicki, Brenner, and Braun



Stern, Dror, Stolovicki, Brenner, and Braun

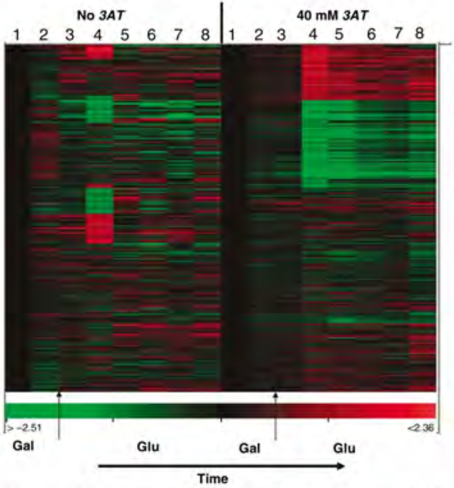


Figure 2 The genome-wide transcription pattern. The raw transcription levels at eight time points for the two experiments, (left) no *3AT*, (right) 40 mM *3AT*, in a color code: red—induced, green—repressed. There are a total of 4148 genes that passed all filters (see Materials and methods). The medium switch from galactose to glucose is marked and the numbers above the columns are the measurement points as shown in Figure 1. Note the differences between the patterns of expression for the two experiments (rows correspond to the same gene in both experiments).

- **the system finds a transcriptional state with many changes**
- **two realizations of the experiment yield vastly different solutions**
- **the same dynamical system seems to have chosen a different attractor** which is then inherited over many generations

If this interpretation is confirmed, we are facing a dynamics in a complex landscape

with the added element of selection

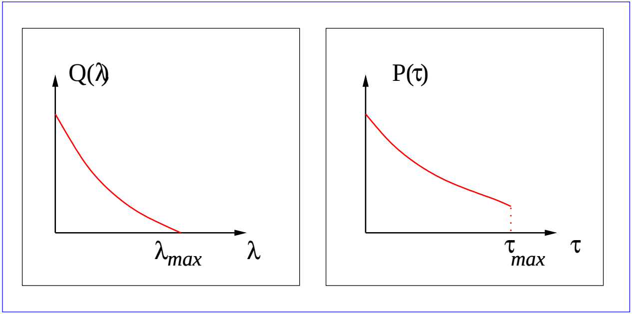
but note that fitness does not drive the dynamics, it acts on its results

the landscape is not the ‘fitness landscape’

A model

T Brotto, G Bunin, JK

M individuals. Attractors with timescale τ_a and reproduction rate λ_a



Without selection pressure the population reaches a finite (smallish) $\langle \tau \rangle$

As soon as the λ_i are turned one, the stationary state dissappears

$\langle \tau \rangle \to \infty$, **and** $\lambda \sim \lambda_{max}$

Evolution of attractor lifetime

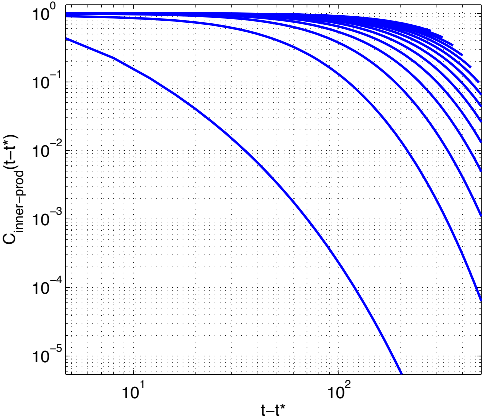
- $\langle\tau\rangle(t) \sim t$ if $P(\tau) \sim \tau^{-\alpha}$ a power law with $\alpha > 2$
- $\langle\tau\rangle(t) \sim t^{\frac{1}{2}}$ if $P(\tau) \sim e^{-a\tau}$
- $\langle\tau\rangle(t) \sim t^{\frac{1}{3}}$ if $P(\tau) \sim e^{-a\tau^2}$

Population divergence time

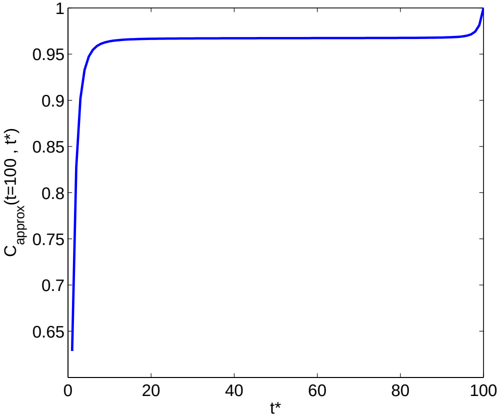
fitness/mutation-rate (anti)correlation

- $t_{div} \sim t$ if $P(\tau) \sim \tau^{-\alpha}$ a power law with $\alpha > 2$
- $t_{div} \sim t^2$ if $P(\tau) \sim e^{-a\tau}$,
- $t_{div} \sim t^3$ if $P(\tau) \sim e^{-a\tau^2}$,

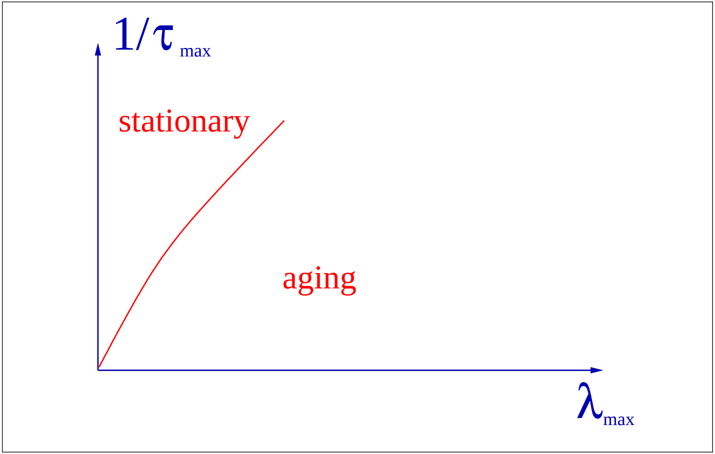
Aging curves



Fraction of population at t born before t^*



How can we understand this anti-intuitive result?



- **Most of the population stays in states with untypically large stability**

- **Average fitness *of the population* hardly improves with time**

- **At large times, lineages present at the beginning manifest themselves!**

- **We may understand this from the large-deviation point of view**