Folding funnel:
A rigorous definition and the fun(nels) it brings.

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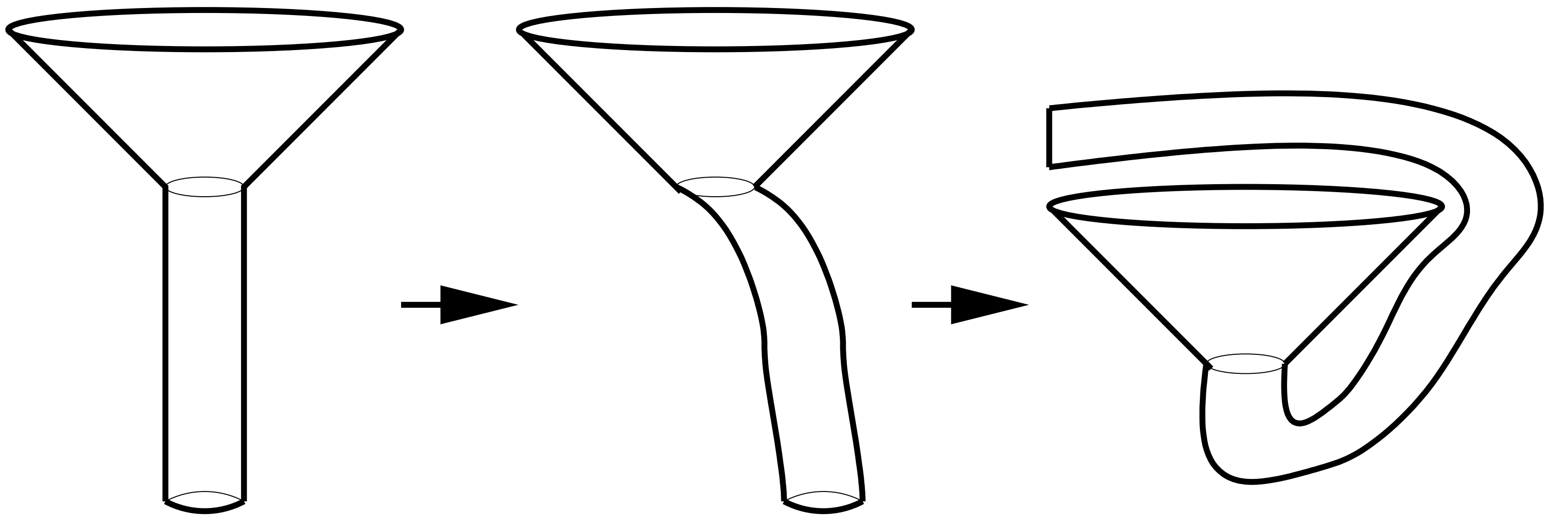
Folding funnel??



Dynamics on a discrete landscape

We define an energy landscape over a state space X by an energy function E and a move set M

$$E : X \to \mathbb{R}, M : X \to \mathcal{P}(X - \{x\})$$

Transition probabilities (Metropolis dynamics)

$$p(y|x) = \frac{1}{|M(y)|} \min\{1, \exp(-\beta(E_y - E_x))\} \qquad \text{for } y \in M(x)$$

and

$$p(x|x) = 1 - \sum_{y \in M(x)} p(y|x)$$

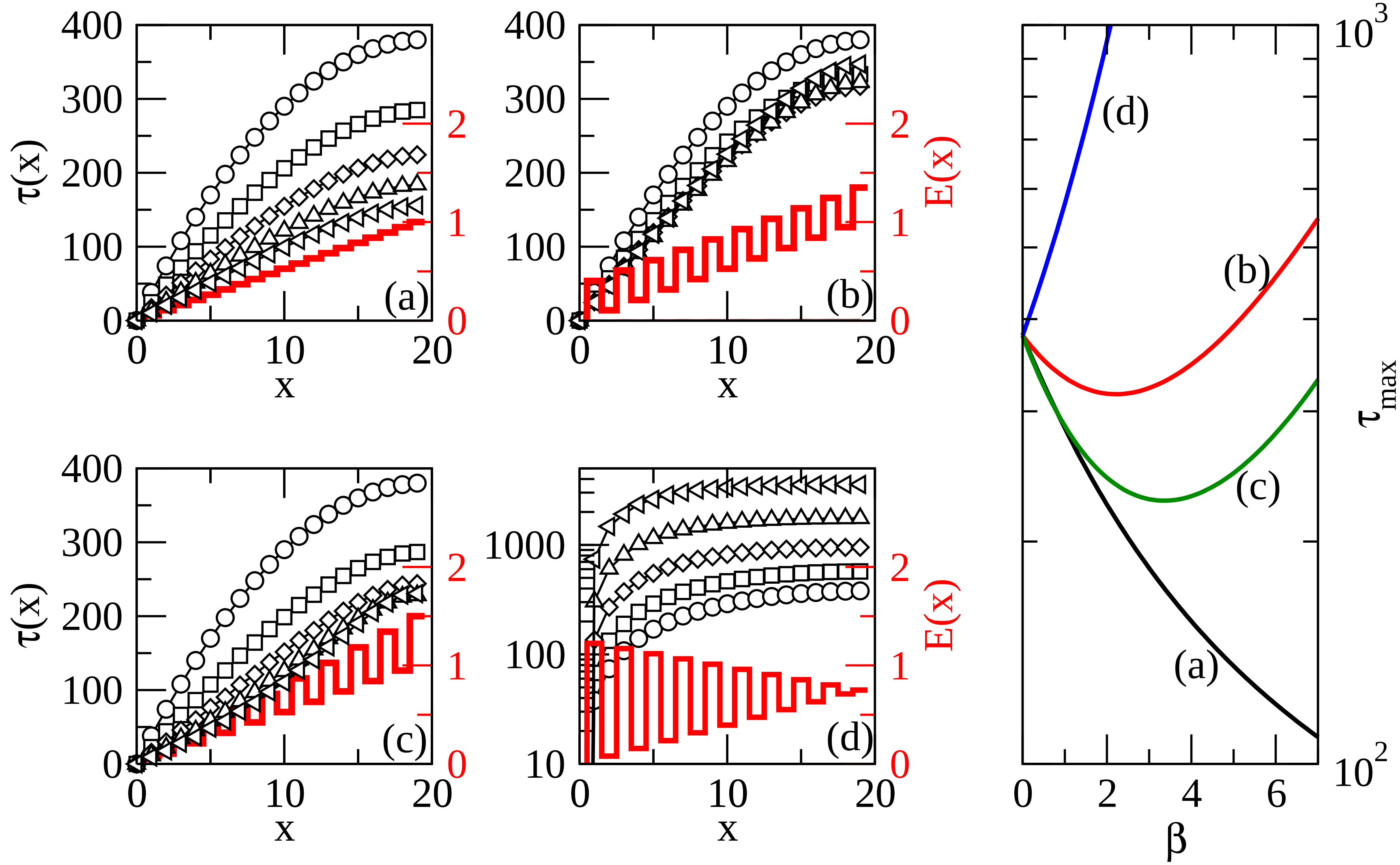
Average time to target

Expected times τ_x it takes to go from a state x to a target state fulfill

$$\tau_x = \sum_{y \in M(x) \cup \{x\}} p(y|x)\tau_y + 1 \ .$$

with $\tau_0 = 0$ (target state).

Time to target in one dimension



Intuitive description of a funnel (now seriously)

- The system leaves the basin of a local minimum via the lowest saddle with the highest probability (neglecting entropy effects).

- Rough deterministic approximation of the dynamics: Jump to the minimum reachable over the lowest saddle. Iterate this.

- Folding funnel: Set of all starting states (structures) from which the sequence of steps over the lowest saddles eventually leads to the ground state.

Geometric definition of a funnel

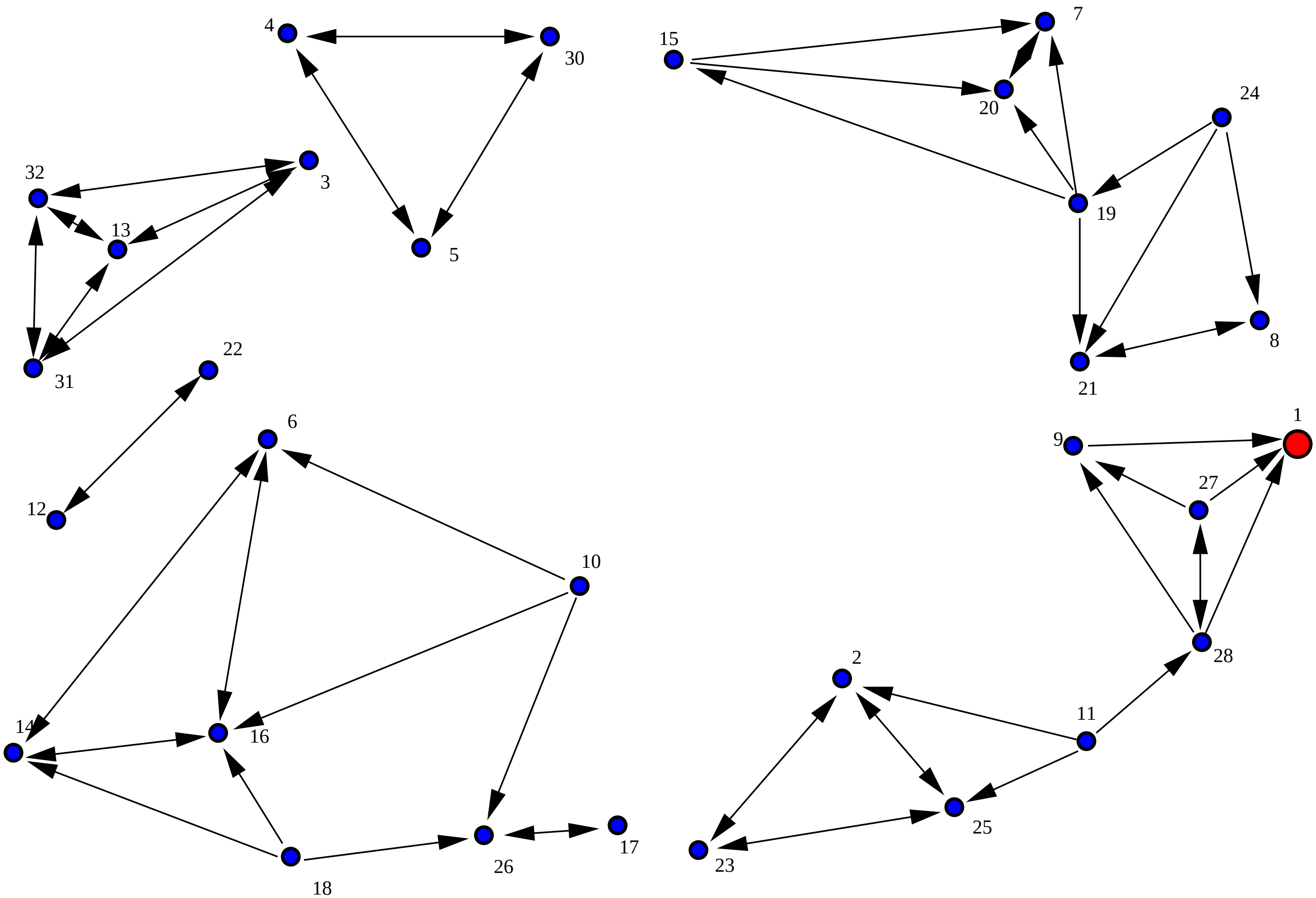
Define *the funnel* recursively as the following set F of states:

1. (1) The ground state is contained in F.

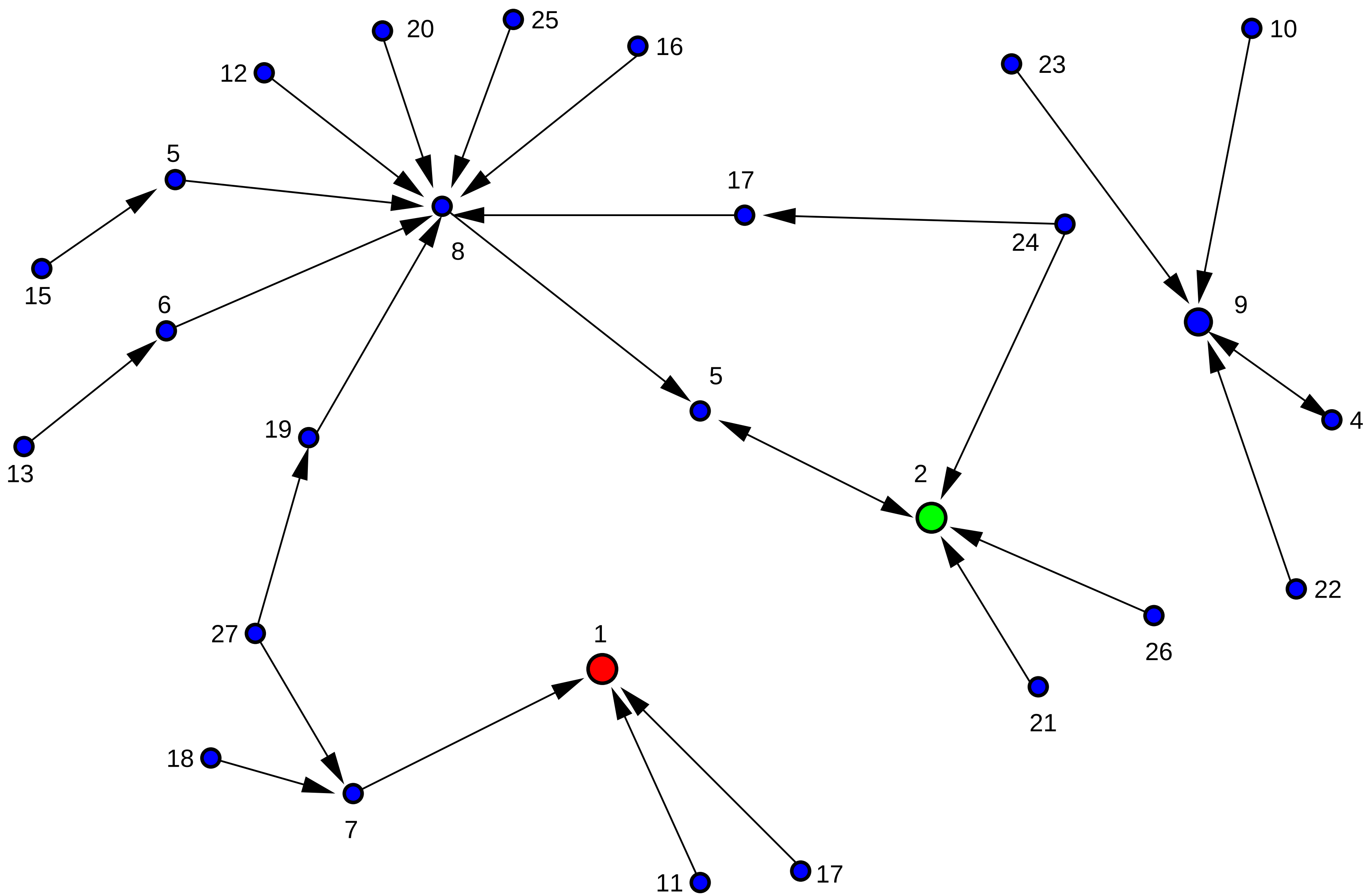
2. (2) The local minimum x belongs to funnel F if a minimum saddle connects it directly to local minimum in the funnel F.

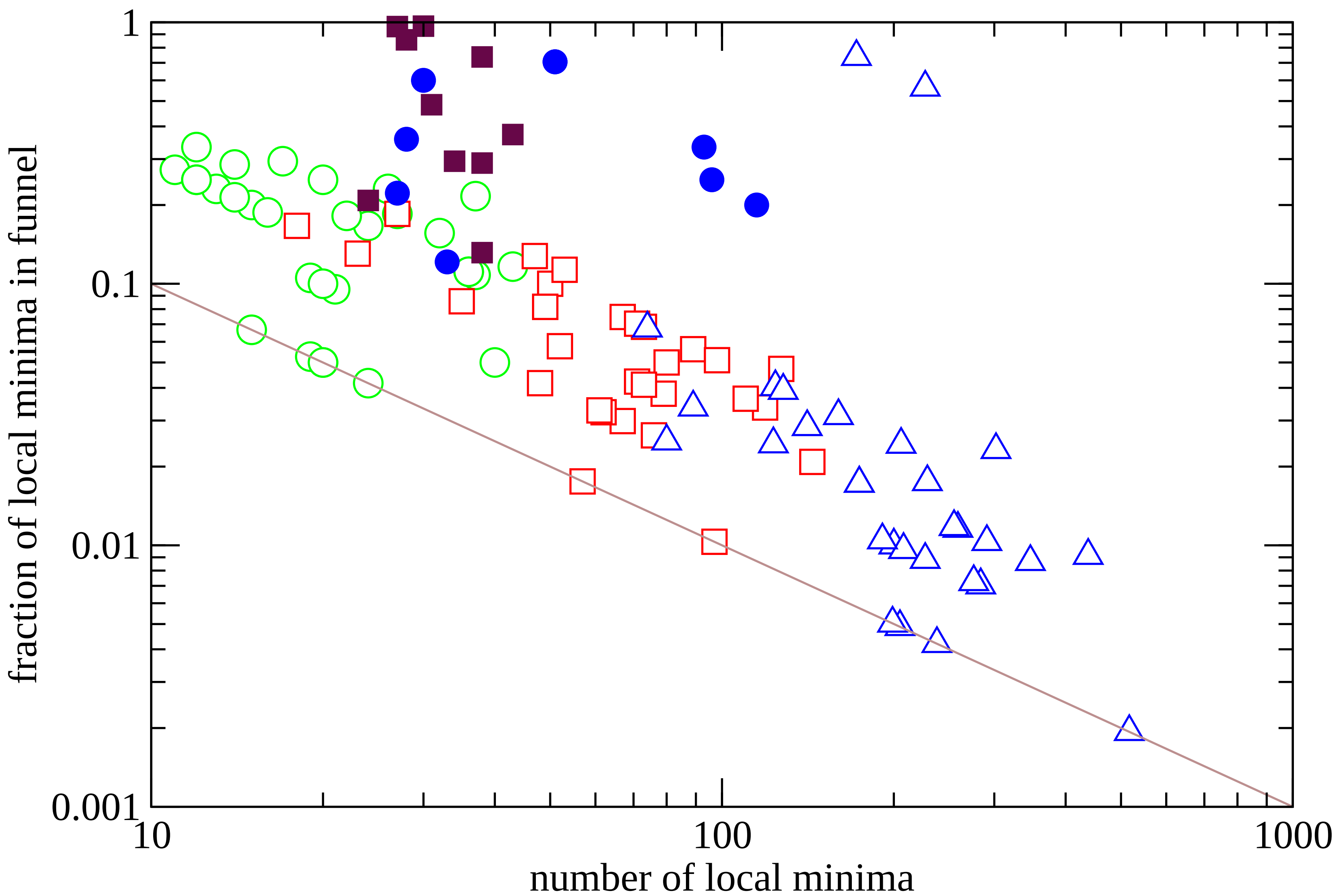
3. (3) A state z belongs to the funnel if it is connected by a gradient descent path to a local minimum in F.

A random instance of the NPP problem



The funnels of xbix





1
0.1
0.01
0.001
10
100
1000
fraction of local minima in funnel
number of local minima