# The Blessing and the Curse
## of the Multiplicative Updates

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# Definition of multiplicative updates

- Algorithm maintains a weight vector
- Weights multiplied by non-negative factors
- Motivated by relative entropies as regularizer

# Machine learning vs nature

Typical multiplicative update in ML

- Set of experts predict something on a trial by trial basis
- $s_i$ is belief in of $i$th expert at trial $t$
- Update: [V,LW]

$$s_i := \frac{s_i\, e^{-\eta \text{loss}_i}}{Z} \qquad \text{where } \eta \text{ learning rate and } Z \text{ normalizer}$$

- Bayes rule is special case

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Nature

- Weights are concentrations / shares in a population

# Multiplicative updates

Blessing

- *Speed*

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for preventing the curse

and discuss related methods used in nature

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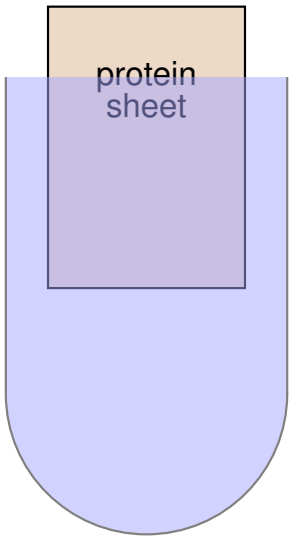
- Next: implementation of Bayes in the tube

# *In-vitro* selection algorithm

- for finding RNA strand that binds to protein

Make tube of *random* RNA strands




for t=1 to 20 do

1. Dip sheet coated with protein into tube
2. Pull out and wash off RNA that stuck
3. Multiply washed off RNA back to original amount (normalization)

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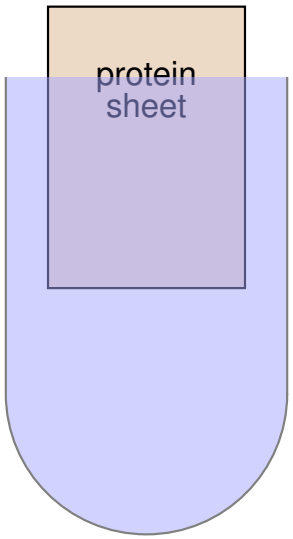


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1. Dip sheet coated with protein into tube
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Can't be done with computer
because $10^{15}$ RNA strands per liter of soup

# Basic scheme

Start with unit amount of random RNA

Loop

1. Functional separation into
   good RNA and bad RNA
2. Amplify good RNA to unit amount

# Duplicating DNA with PCR

## needed for normalization step

- Invented by Kary Mullis 1985
- Heat - double stranded DNA comes apart
- Cool - Short primers hybridize at the ends
- Taq Polymerase runs along DNA strand and complements bases
- Back to double stranded DNA

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- Ideally all DNA strands multiplied by factor of 2

# The caveat

- Not many interesting/specific functional separations found
- Need high throughput for functional separation

# Mathematical description of in-vitro selection

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Strong assumption:

- Fitness $W_i$ independent of share vector $\boldsymbol{s}$

# Update

Good RNA in tube $\boldsymbol{s}$:

$$s_1 W_1 + s_2 W_2 + \cdots + s_n W_n = \boldsymbol{s} \cdot \boldsymbol{W}$$

Bad RNA:

$$s_1(1 - W_1) + s_2(1 - W_2) + \cdots + s_n(1 - W_n) = 1 - \boldsymbol{s} \cdot \boldsymbol{W}$$

- Amplification:
  - Good share of RNA $i$ is $s_i W_i$ - multiplied by factor $F$
  - If precise, then all good RNA multiplied by same factor $F$
  - Final tube at end of loop

$$F\ \boldsymbol{s} \cdot \boldsymbol{W}$$

  - Since final tube has unit amount of RNA

$$F\ \boldsymbol{s} \cdot \boldsymbol{W} = 1 \text{ and } F = \frac{1}{\boldsymbol{s} \cdot \boldsymbol{W}}$$

  - Update in each loop

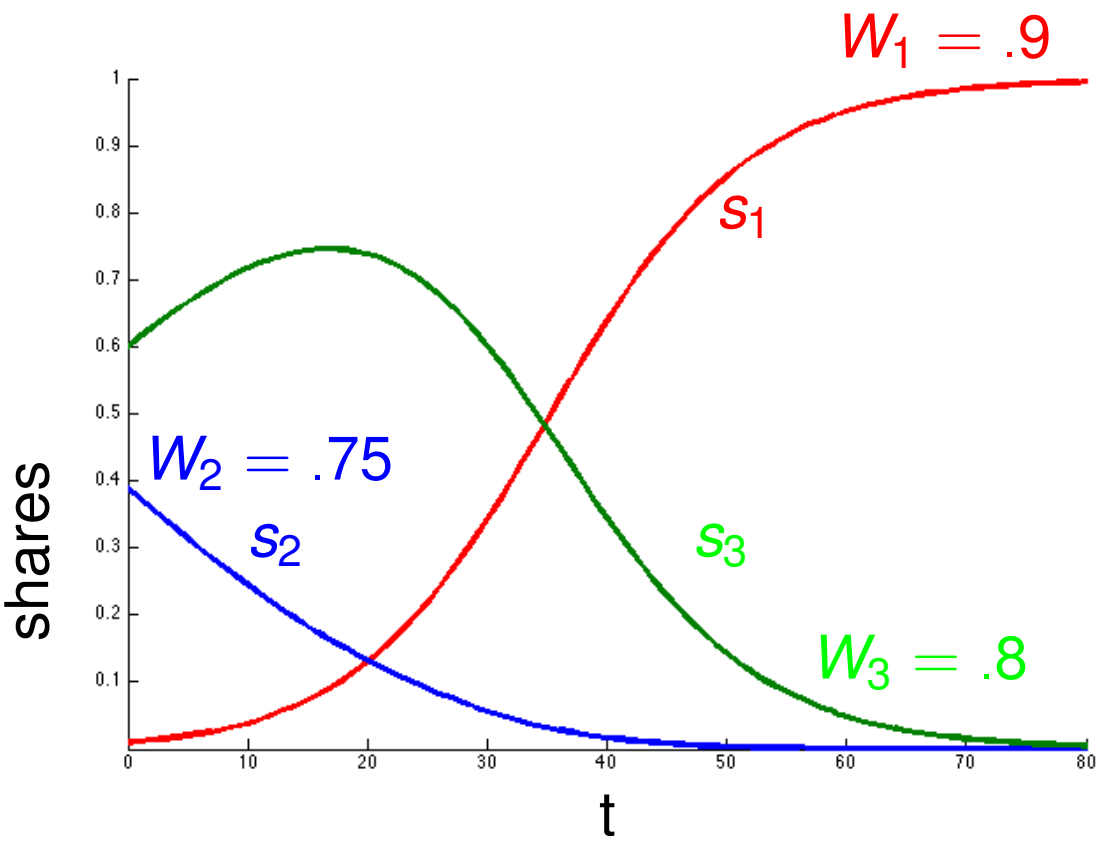
$$s_i := \frac{s_i W_i}{\boldsymbol{s} \cdot \boldsymbol{W}}$$

# Implementing Bayes rule in RNA

- $s_i$ is prior $P(i)$
- $W_i \in [0..1]$ is probability $P(Good|i)$
- $\boldsymbol{s} \cdot \boldsymbol{W}$ is probability $P(Good)$
-

$$s_i := \frac{s_i W_i}{\boldsymbol{s} \cdot \boldsymbol{W}} \quad \text{is Bayes rule} \quad \underbrace{P(i|Good)}_{\text{posterior}} = \frac{\overbrace{P(i)}^{\text{prior}} P(Good|i)}{P(Good)}$$

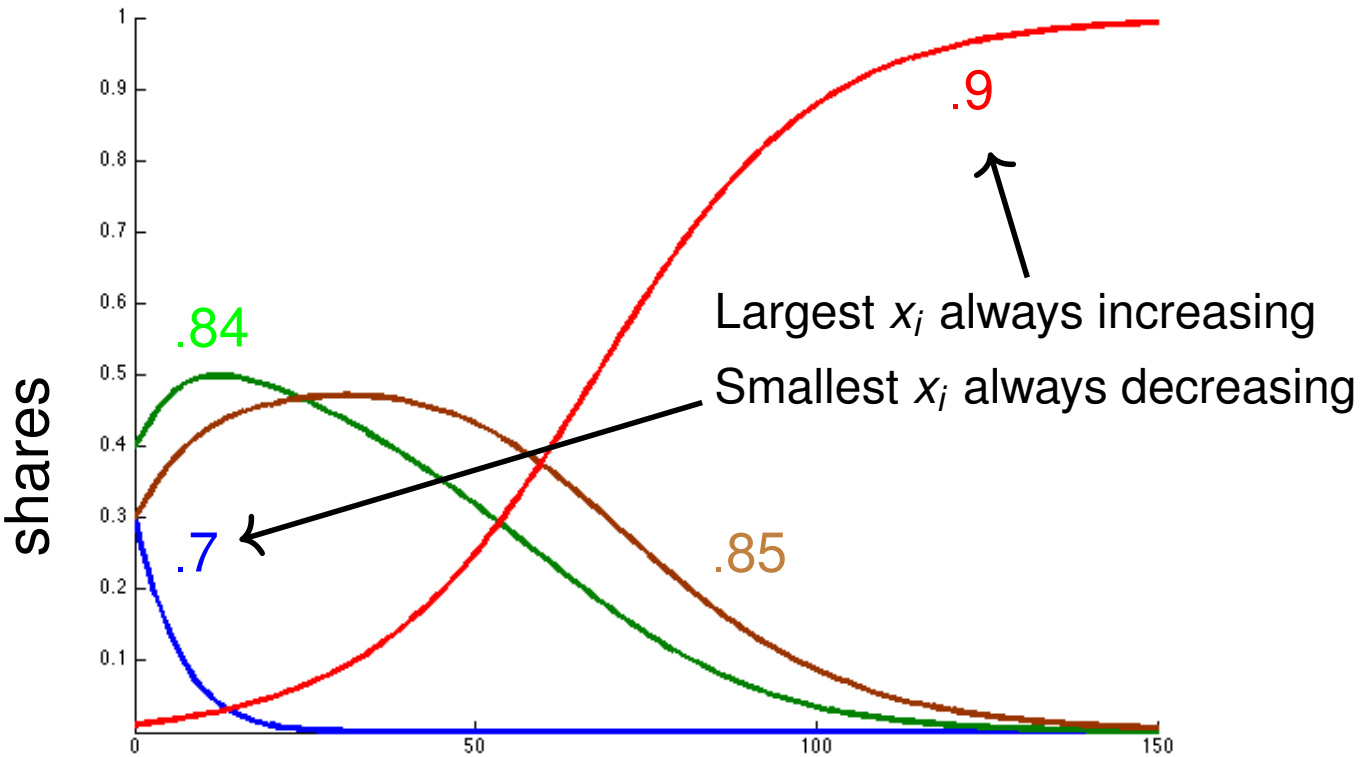
# Iterating Bayes Rule with same data likelihoods




Initial $\boldsymbol{s} = (.01, .39, .6)$

$\boldsymbol{W} = (.9, .75, .8)$

# $\max_i W_i$ eventually wins




$$s_{t,i} = \frac{s_{0,i} W_i^t}{\text{normalization}}$$

$t$ is speed parameter

# The best are *too* good

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$$s_i \sim s_i \underbrace{\text{fitness factor}_i}_{\geq 0}$$

- Blessing

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  Can do this with $10^{15}$ variables

- Curse

  The best wipe out the others
  Loss of diversity

# View of evolution

Simple view

- Inheritance
  - mutation
  - selection for the fittest with multiplicative update

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Different view

- Multiplicative updates are brittle
- A mechanism is needed to ameliorate the curse of the multiplicative update
- Machine Learning and Nature uses various mechanisms

# Another tube experiment

Tube with nutrient solution

- Add 100 different bacteria and wait
- How many survive?

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Same experiment but agitate tube

- How many survive
- One - because only one niche left

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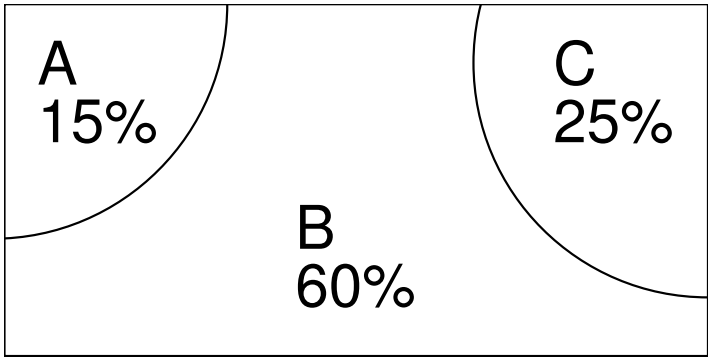
Why is this bad?

# A first key problem

## that cannot be solved by multiplicative update alone

- 3 strands of RNA
- Want to amplify mixture while keeping percentages unchanged



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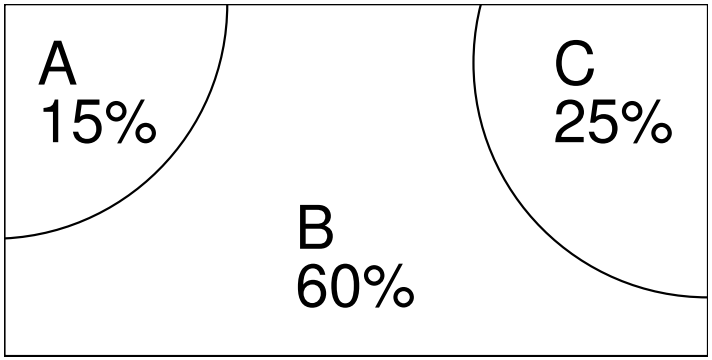


Iterative amplification will favor one!

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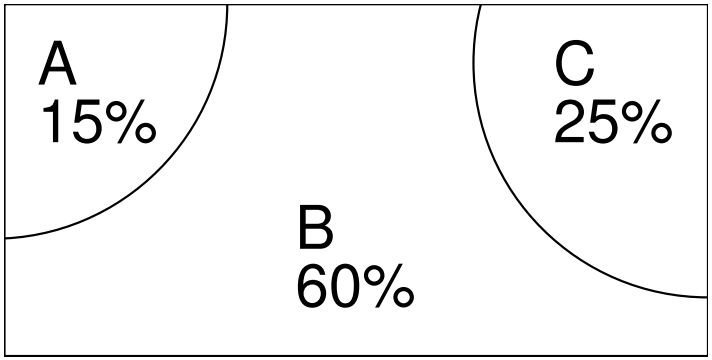


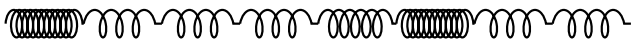

Iterative amplification will favor one!

Fitness factor $W_i$
- ideally all equal 2
- not the same to high precision
- dependant on the concentrations

# Solution

- Make one long strand with roughly right percentages of A,B,C

  A B B B C A B B



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- Chop into constituents
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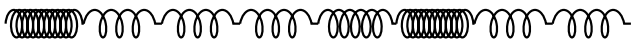

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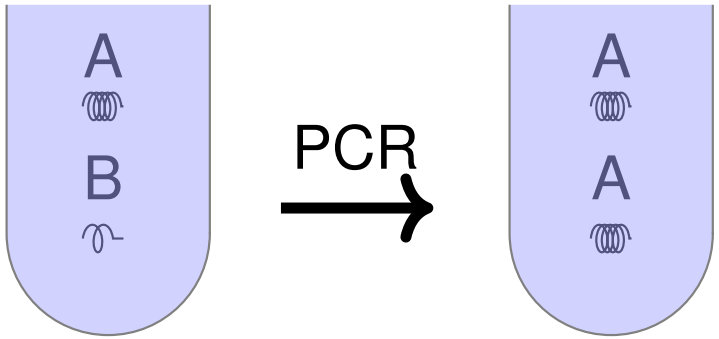
Big picture

- Long strand functions as "chromosome"
  - Free floating genes in the nucleus would compete
  - Loss of diversity

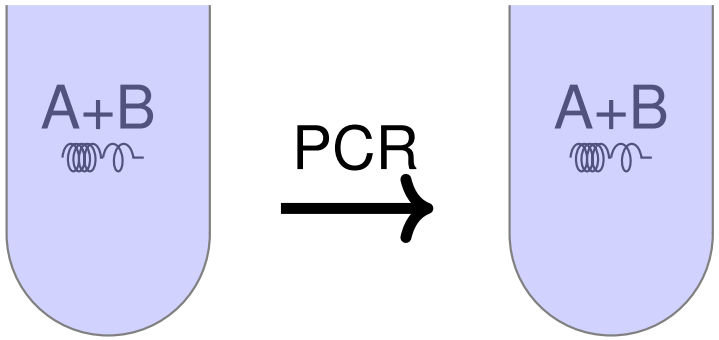
# Nature 2: Coupling preserves diversity

Un-coupled




A and B compete

Coupled




A and B should cooperate

# Many questions already about in-vitro selection

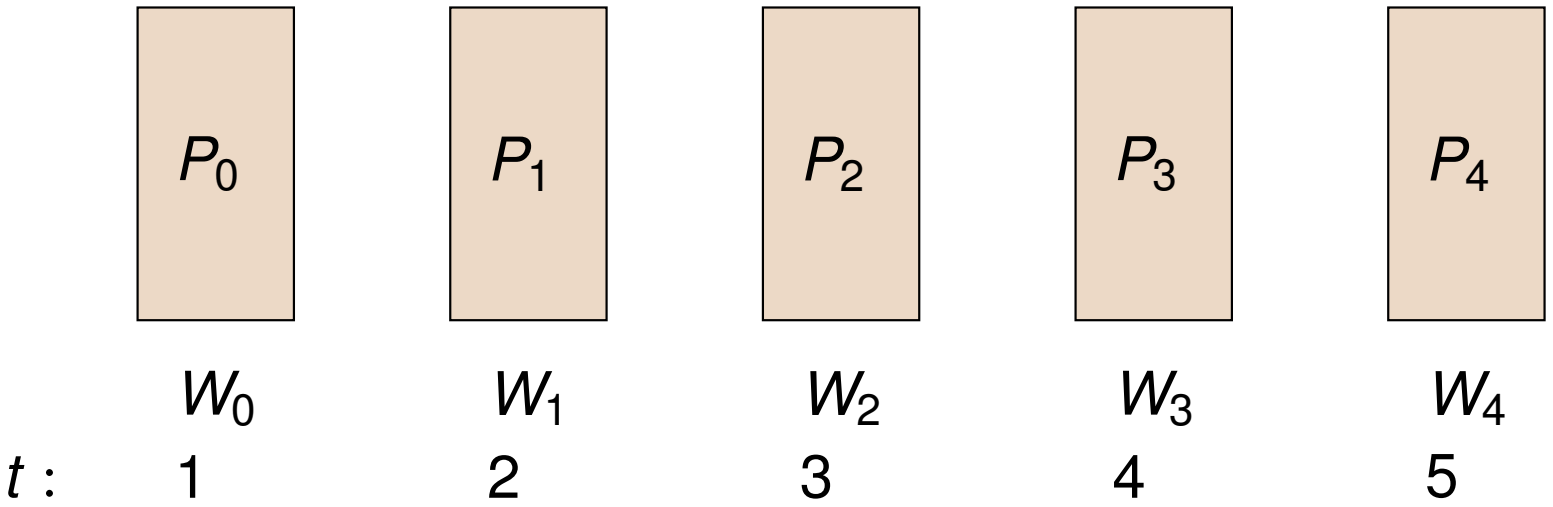
- a bare-bones evolutionary process

- What updates to $\boldsymbol{s}$ represent an iteration of an in-vitro selection update?
- What updates are possible with blind computation?
- Must maintain non-negative weights

# A second problem

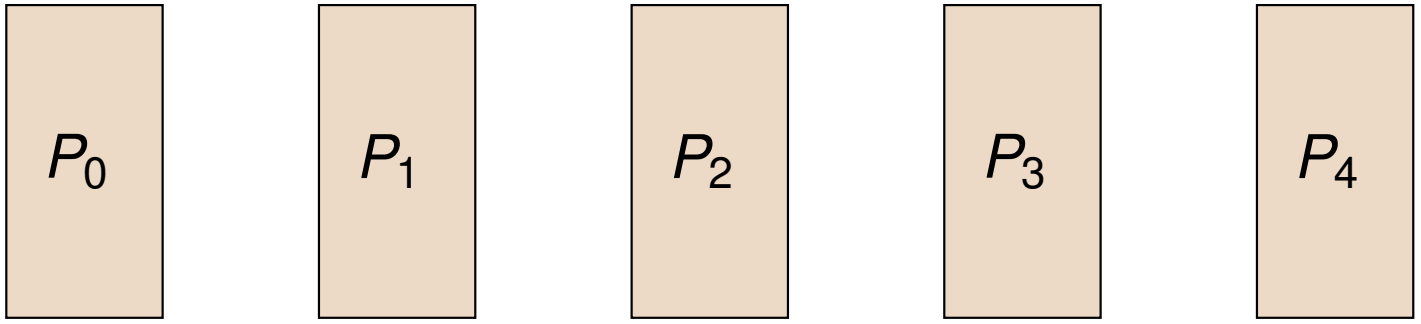
- that also cannot solved by just a multiplicative update

Find set of RNA strands that binds to a $q$ different proteins $W_j$




- In trial $t$, functional separation based on fitness vector $\boldsymbol{W}_{t \mod q}$
- So far all $\boldsymbol{W}_j$ the same

# In-vitro selection algorithm




| | | | | | |
|---|---|---|---|---|---|
| $W_{j,1}$ | 0.9 | 0.8 | 0.96 | 0.2 | 0.04 |
| $W_{j,2}$ | 0.1 | 0.01 | 0.8 | 0.9 | 0.8 |

# In-vitro selection algorithm

| | $P_0$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ |
|---|---|---|---|---|---|
| $W_{j,1}$ | 0.9 | 0.8 | 0.96 | 0.2 | 0.04 |
| $W_{j,2}$ | 0.1 | 0.01 | 0.8 | 0.9 | 0.8 |
| $\boldsymbol{u} \cdot \boldsymbol{W}_j$ | 0.5 | 0.405 | 0.88 | 0.55 | 0.42 |

## Goal Tube

Tube: $\boldsymbol{u} = (0.5, 0.5, 0, \ldots, 0)$

The two strands cooperatively solve the problem
Related to disjunction of two variables

# Key problem 2

## Goal

Starting with 1 liter tube in which all strands appear with frequency $\approx 10^{-15}$, use PCR and . . . , to arrive at tube :

$$(\approx 0.5, \approx 0.5, \approx 0, \ldots, \approx 0)$$

- Problem
  - Over train with $P_0$ and $P_1 \Rightarrow s_1 \approx 1, s_2 \approx 0$
  - Over train with $P_3$ and $P_4 \Rightarrow s_1 \approx 0, s_2 \approx 1$
- Want blind computation!
  - $\boldsymbol{W}_j$ and initial $\boldsymbol{s}$ unknown
- Need some kind of feedback in each trial

# Related machine learning problem

- Tube $\equiv$ share vector $\boldsymbol{s} \in$ probability simplex$^N$
- Proteins $\equiv$ Example vectors $\boldsymbol{W}_t \in \{0,1\}^N$

## Assumption

$\exists \boldsymbol{u} = (0, 0, \frac{1}{k}, 0, 0, \frac{1}{k}, 0, 0, \frac{1}{k}, 0, 0, 0)$
with $k$ non-zero components of value $\frac{1}{k}$
s.t. $\forall t : \boldsymbol{u} \cdot \boldsymbol{W}_t \geq \frac{1}{k}$

## Goal

Find $\boldsymbol{s} : \boldsymbol{s} \cdot \boldsymbol{W}_t \geq \frac{1}{2k}$

# Normalized Winnow Algorithm (N. Littlestone)

Do passes over examples $\boldsymbol{W}_t$

if $\underbrace{\boldsymbol{s}_{t-1} \cdot \boldsymbol{W}_t}_{\text{good side}} \geq \frac{1}{2k}$

$$\text{then} \quad \boldsymbol{s}_t := \boldsymbol{s}_{t-1} \qquad \text{conservative update}$$

$$\text{else} \quad s_{t,i} := \begin{cases} s_{t-1,i} & \text{if} \quad W_{t,i} = 0 \\ \alpha s_{t-1,i} & \text{if} \quad W_{t,i} = 1, \quad \text{where } \alpha > 1 \end{cases}$$

and re-normalize

- $O(k \log \frac{N}{k})$ updates needed
  when labels consistent with $k$-literal disjunction
- Logarithmic in $N$
- Optimal to within constant factors

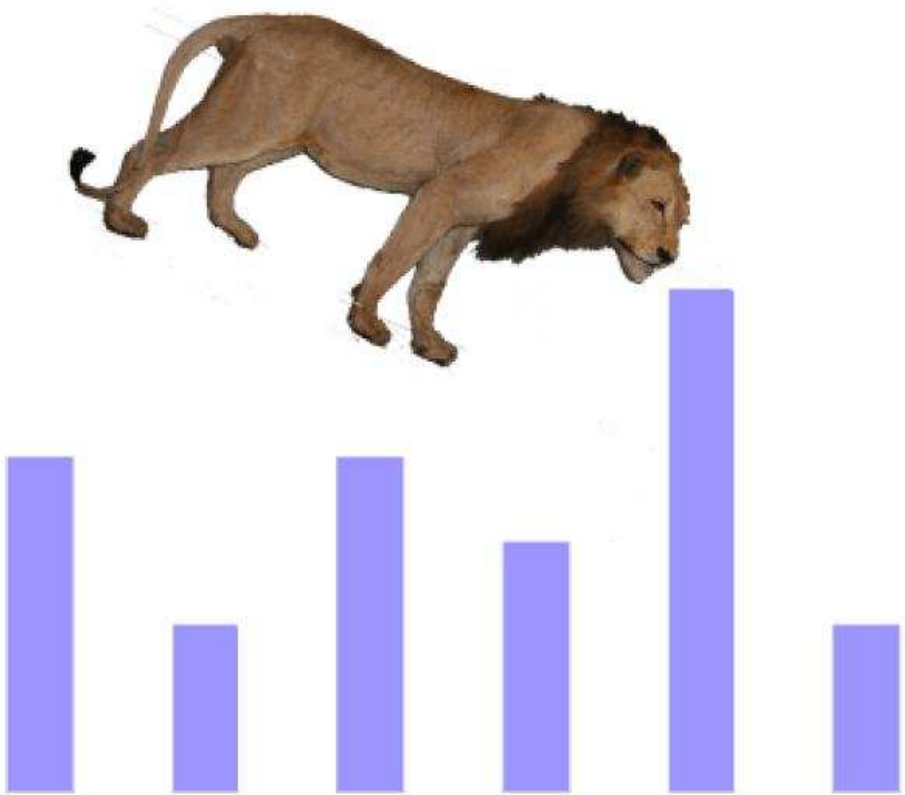
# ML 1: prevent overtraining with conservative update

- Assume we can measure the dot product $\boldsymbol{s}_{t-1} \cdot \boldsymbol{W}_t$ i.e. a concentration of RNA strands,
- then normalized Winnow can be implemented with Blind Computation
- Algorithms uses $n$ weights to learn $\binom{n}{k}$ concepts
- Coupling is replaced by thresholding

## Next trick

Cap weights
- Start with nature
- How we used same trick in Machine learning

# Nature 3: Super predator



Preserves diversity

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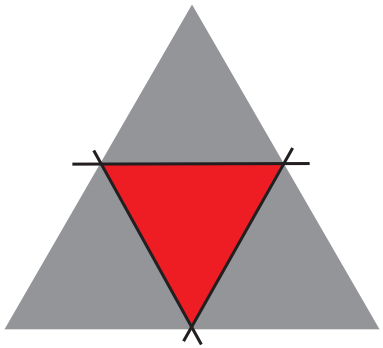
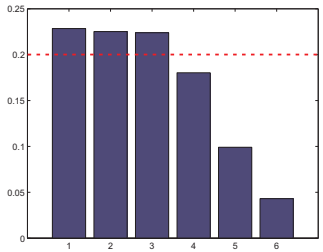
# ML 2: cap weights

$$s'_i = \frac{s_i \; e^{-\eta \; Loss_i}}{Z}$$

$$\boldsymbol{s} = \text{capped and rescaled version of } \boldsymbol{s}'$$

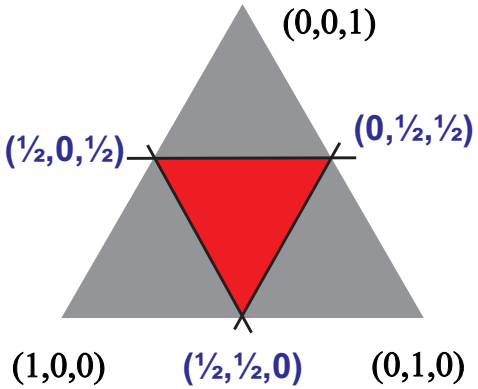


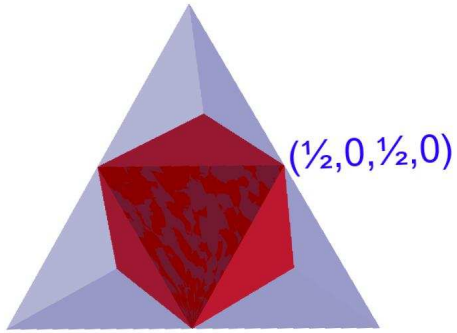



Cap and re-scale rest

# Why capping?

- $m$ sets encoded as probability vectors $(0, \frac{1}{m}, 0, 0, \frac{1}{m}, 0, \frac{1}{m})$ called $m$-corners $\binom{n}{m}$ of them
- The convex hull of the $m$-corners = capped probability simplex




- Combined update converges to best corner of capped simplex - best set of size $m$
- Capping lets us learn multiple goals - learn the best set of experts
- The matrix version of this algorithm leads to the best on-line algorithm for Principal Component Analysis
- How to cap in in-vitro selection setting?

# What if environment changes over time (M. Herbster)

- Initial tube contains $10^{15}$ different strands
- After a while —
  - Loss of diversity
  - Some selfish strand manages to dominate without doing the wanted function

## Fixes

- Mix in a little bit of initial soup for enrichment
- Or do sloppy PCR that introduces mutations

# Disk spindown problem

- Experts a set of $n$ fixed timeouts : $\tau_1, \tau_2, \ldots, \tau_n$
- Master Alg.
  - maintains a set of weights : $s_1, s_2, \ldots, s_n$
  - predicts with weighted average
- Multiplicative update

$$s_{t+1,i} = \frac{s_{t,i}\ \boldsymbol{e}^{-\eta \text{ energy usage of timeout i}}}{Z}$$

- Problem

# Disk spindown problem

- ML 3: Mix in little bit of uniform vector

$$\begin{aligned} \boldsymbol{s}' &= \text{Multiplicative Update} \\ \boldsymbol{s} &= (1-\alpha)\,\boldsymbol{s}' + \alpha\,(\frac{1}{N}, \frac{1}{N}, \ldots, \frac{1}{N}) \\ & \quad \text{where } \alpha \text{ is small} \end{aligned}$$

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- Nature 4: use mutation for same purpose

# ML 4: sleeping

- Keep track of past average share vector $\boldsymbol{r}$

$$\begin{aligned} \boldsymbol{s}' &= \text{Multiplicative Update} \\ \boldsymbol{s} &= (1-\alpha)\,\boldsymbol{s}' + \alpha\,\boldsymbol{r} \end{aligned}$$

- facilitates switch to previously useful vector
- long-term memory

Sleeping interpretation - “Putting Bayes to sleep” [KAW]

- Some models predict with predictive distribution
- Weights of those models fixed - Bayes rule is vacuous

# Two-track in-vitro implementation of sleeping

Multiplicative update + small soup exchange gives long-term memory

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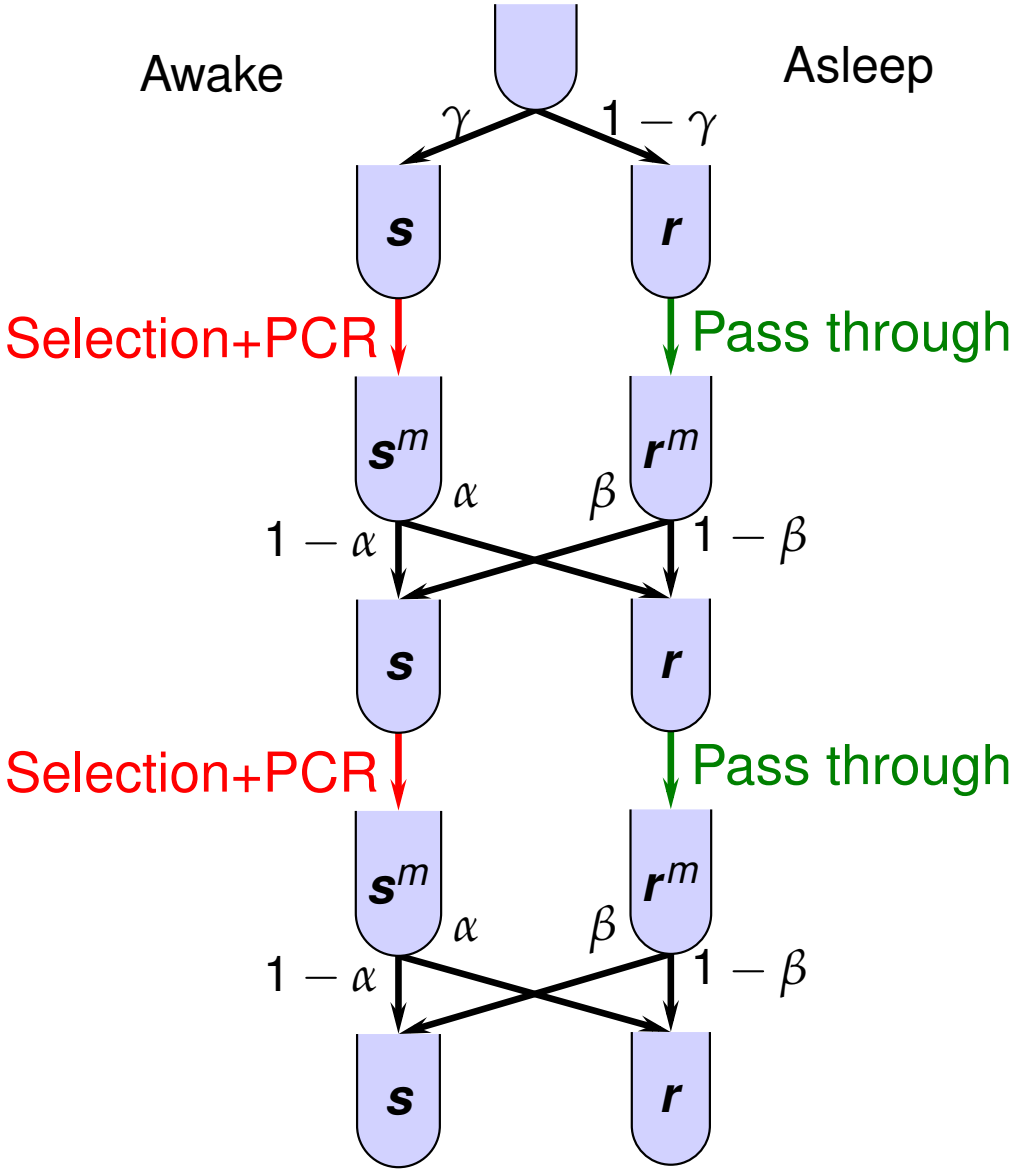

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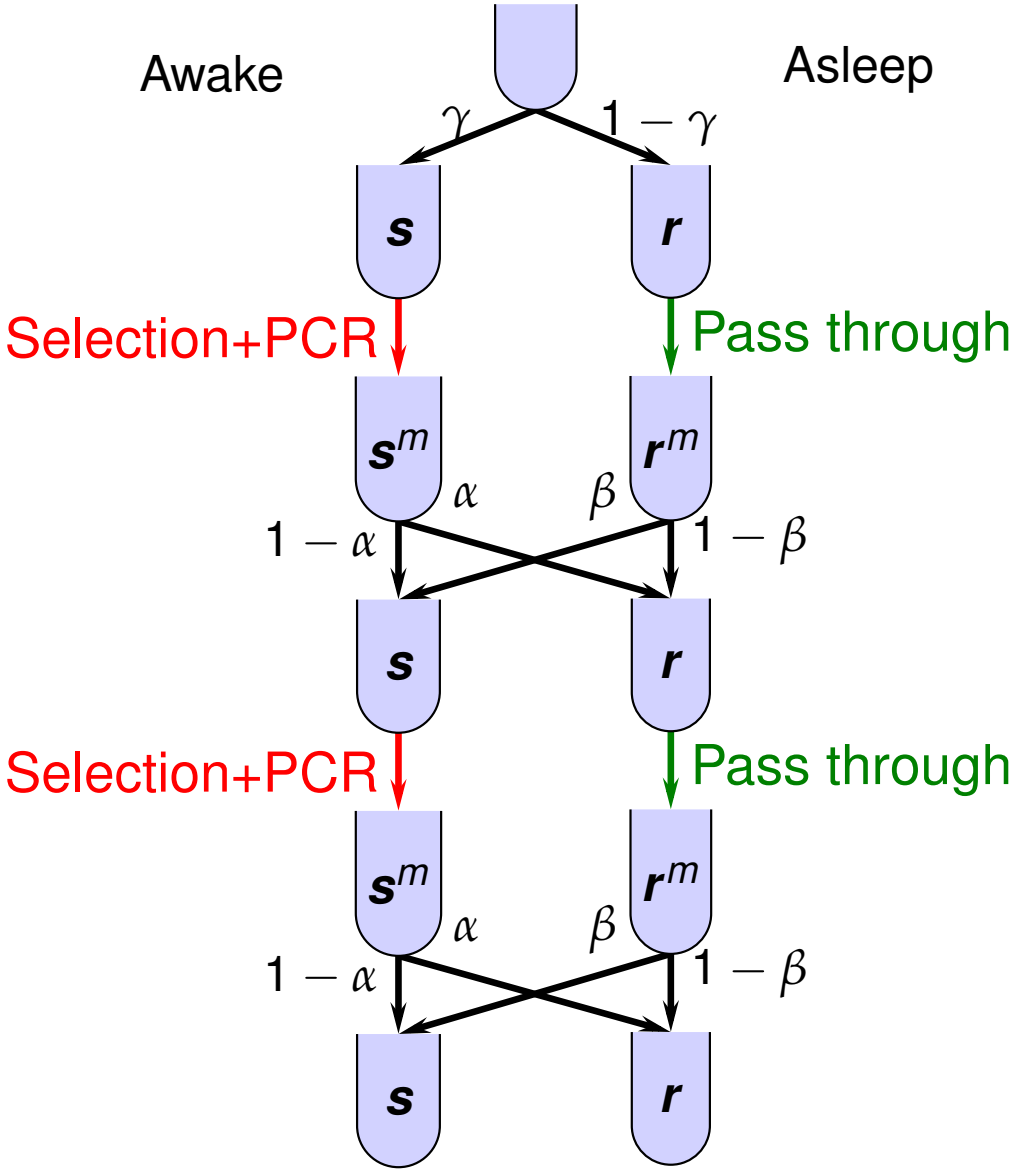



Initially:

$\boldsymbol{s} = \gamma$ "initial tube"

$\boldsymbol{r} = (1-\gamma)$ "initial tube"

$\boldsymbol{s}^m =$ "mult.update"$(\boldsymbol{s})$

$\boldsymbol{r}^m = \boldsymbol{r}$

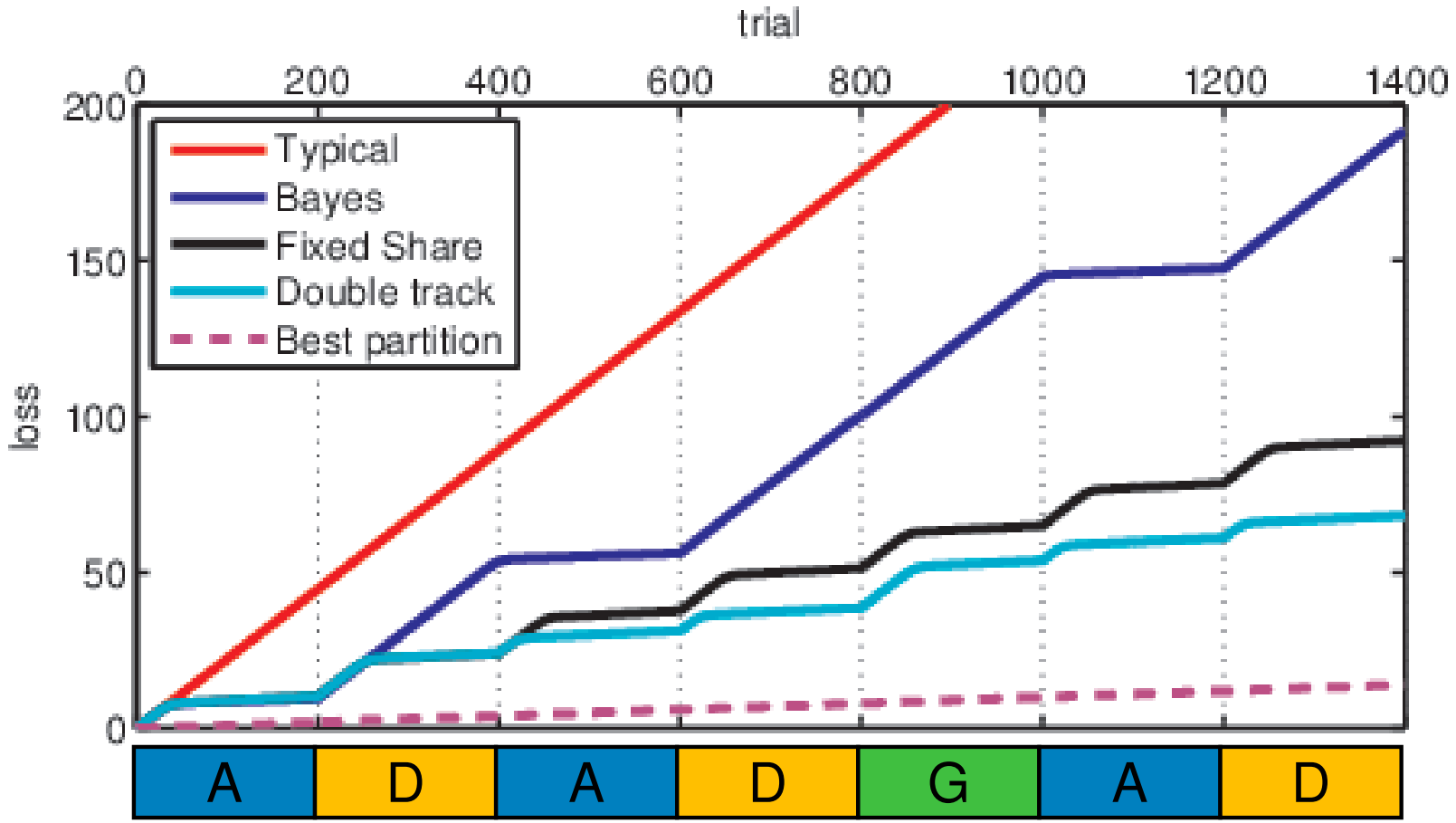
Soup exchange:

$\tilde{\boldsymbol{s}} = (1-\alpha)\boldsymbol{s}^m + \beta \boldsymbol{r}^m$

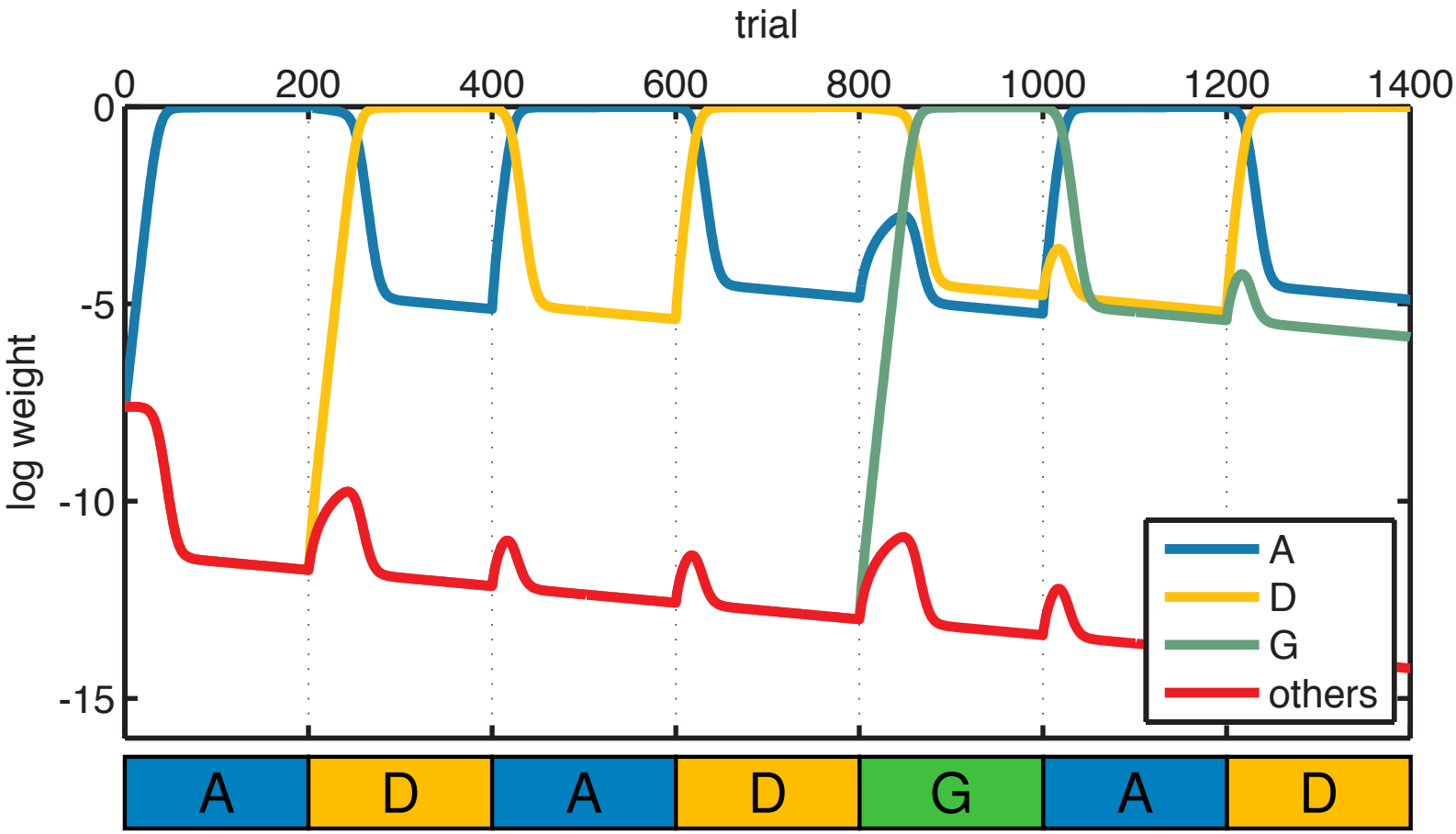
$\tilde{\boldsymbol{r}} = \alpha \boldsymbol{s}^m + (1-\beta)\boldsymbol{r}^m$

$\gamma = \frac{\beta}{\alpha+\beta}$

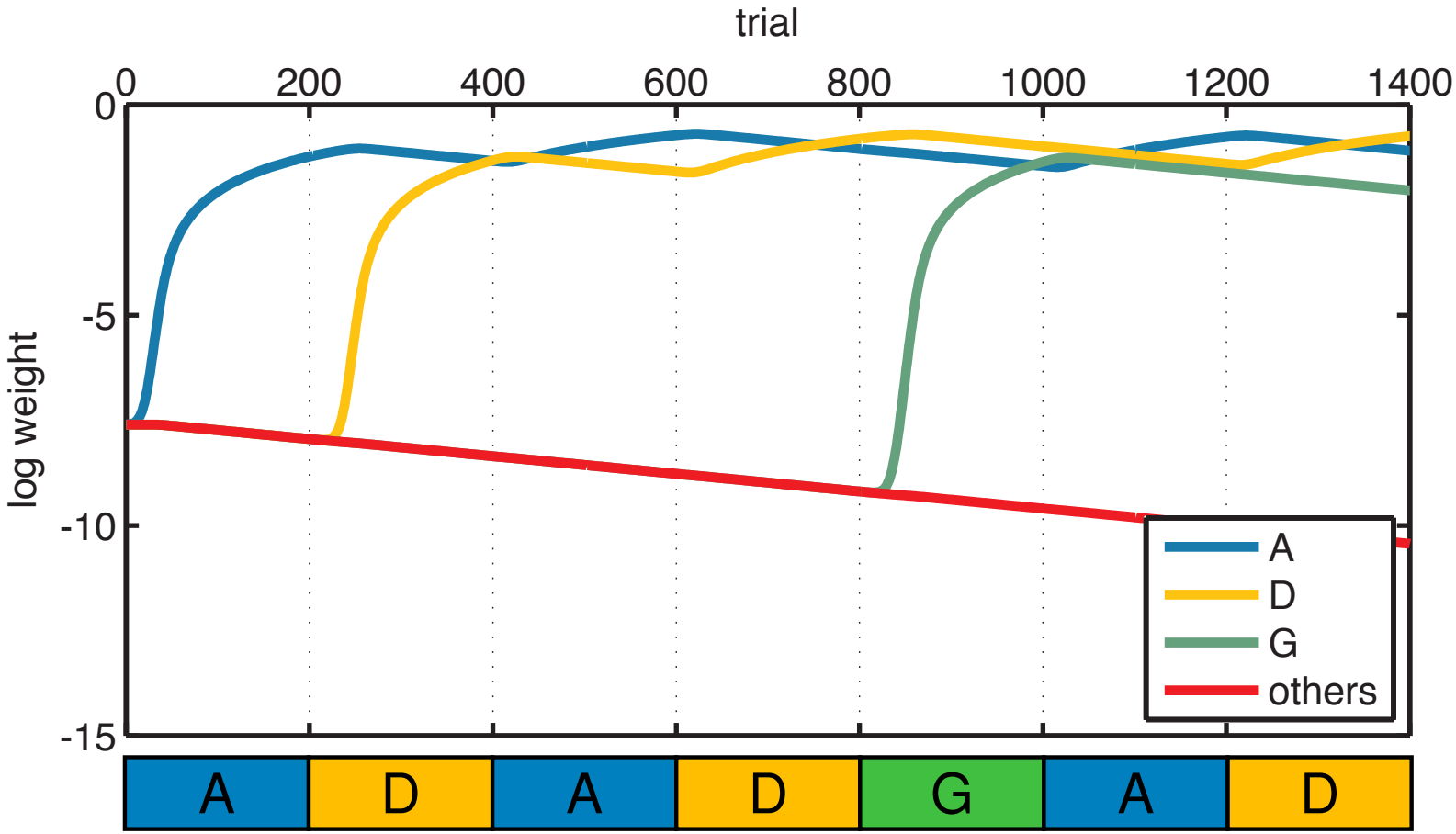
# Total loss plots



# Weights $\boldsymbol{s}$ on the awake track



# Weights *r* on the sleeping track



# Question

- How long-term memory realized in nature?
  - Junk DNA?
  - Sex?

## ML methods

ML 1: Conservative update - learn multiple goals
ML 2: Upper bounding weights - ”
ML 3: Lower bounding weights - robust against change
ML 4: Mixing in past average/sleeping - longterm memory

## Nature’s methods

Nature 1: Boundaries
Nature 2: Coupling
Nature 3: Super-predators
Nature 4: Mutations

# Summary

- Multiplicative updates converge quickly - their blessing but wipe out diversity - their curse
- Changing conditions require reuse of previously learned knowledge/alternatives
- Diversity is a requirement for success
- A mechanism is need to ameliorate the curse
  - ML and Nature have different tricks

# Final question 1

Would three tracks imbue a layered long-term memory

# Final question 2

- Does nature use the matrix version of the multiplicative updates?

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- Does nature use the matrix version of the multiplicative updates?
- Parameter is density matrix
  - maintains uncertainty over directions as symmetric positive matrix $\boldsymbol{S}$

$$\widetilde{\boldsymbol{S}} := \frac{\exp(\log \boldsymbol{S} - \eta \nabla L(\boldsymbol{S}))}{\text{trace of above}}$$

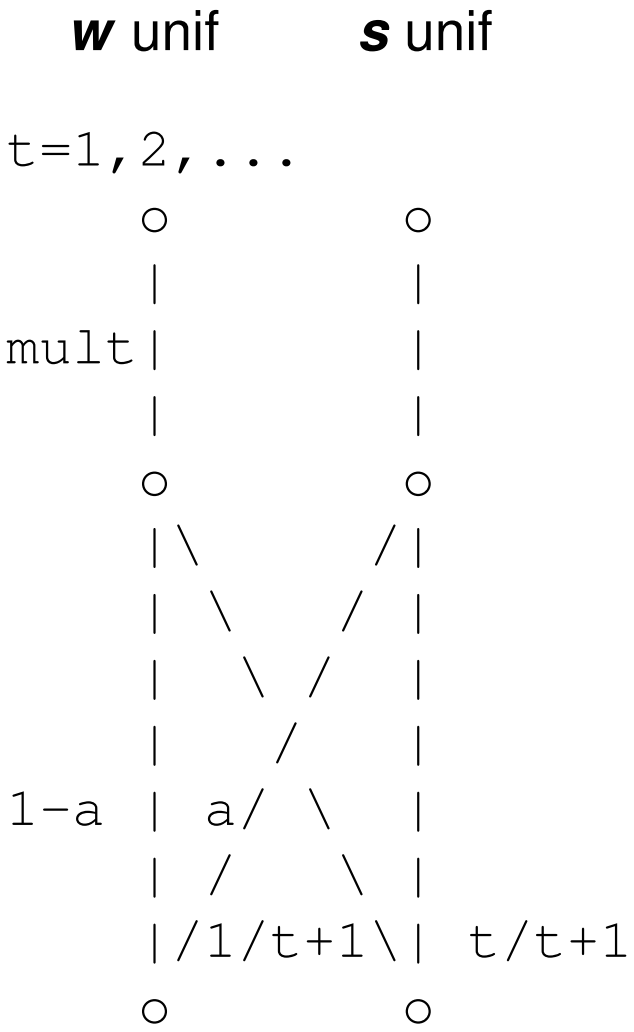
# Final question 2

- Does nature use the matrix version of the multiplicative updates?
- Parameter is density matrix
  - maintains uncertainty over directions as symmetric positive matrix $\boldsymbol{S}$

$$\widetilde{\boldsymbol{S}} := \frac{\mathbf{exp}(\mathbf{log}\boldsymbol{S} - \eta \nabla L(\boldsymbol{S}))}{\text{trace of above}}$$

- Quantum relative entropy as regularizer

# Fixed Share to Uniform Past

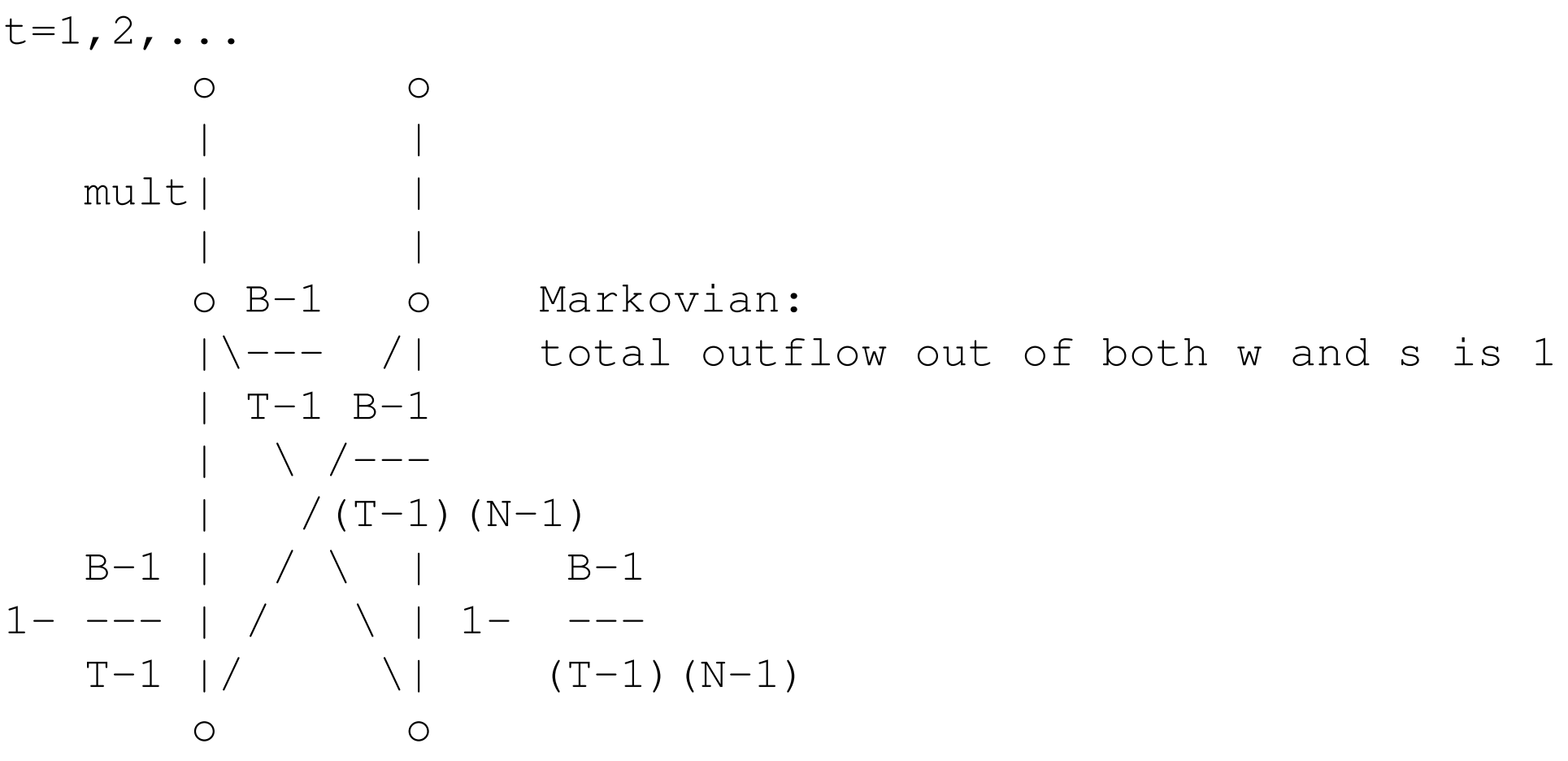



total inflow into w and s is 1

***w*** and ***s*** remain probability vectors

# Fixed Share to Exponentially Decaying Past

Tuned for $B$ shifts in $T$ trials
Shift among small pool of $N$ in large pool of $M$ $\quad \boldsymbol{w} = (\frac{1}{M}, \ldots, \frac{1}{M})\frac{1}{N}$
$\boldsymbol{s} = (\frac{1}{M}, \ldots, \frac{1}{M})(1 - \frac{1}{N})$

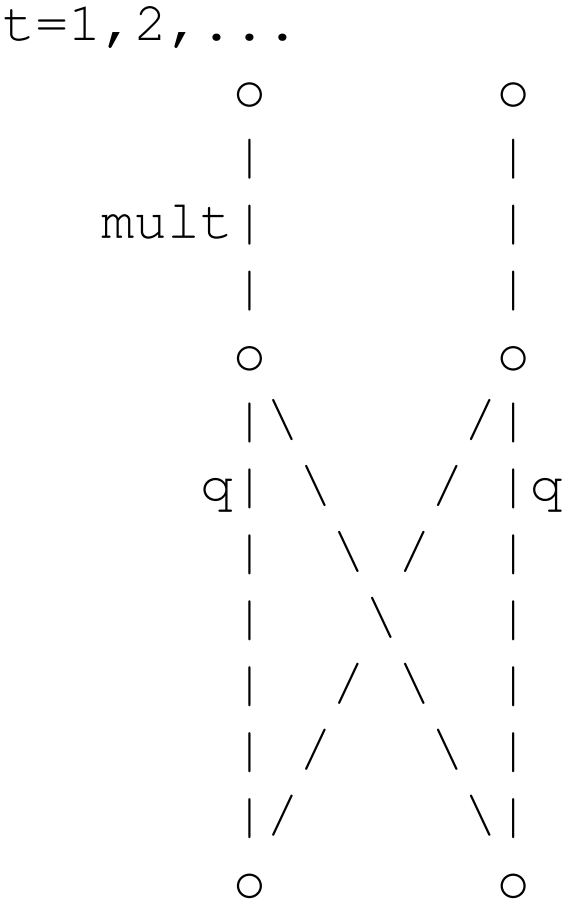



$\boldsymbol{w}$ and $\boldsymbol{s}$ remain at total weight $\frac{1}{N}$ and $1 - \frac{1}{N}$, resp.

# Fixed Share to Exponentially Decaying Past

Number of segments $B$ and horizon $T$ unknown

$\boldsymbol{w} = \frac{\text{unif}}{2}$ $\quad$ $\boldsymbol{s} = \frac{\text{unif}}{2}$




Markovian:
total outflow out of both w and s is 1

where $q = exp(-\frac{1}{t \ln^2(t+1)})$

$\boldsymbol{w}$ and $\boldsymbol{s}$ remain at total weight $\frac{1}{2}$