ESTIMATION OF DISTRIBUTION ALGORITHMS

Estimation of distribution algorithms (EDAs) are a class of probabilistic optimization algorithms that model the search distribution of candidate solutions in the search space. The basic idea behind EDAs is to build a probabilistic model of promising solutions based on the information gathered from the current population and use this model to guide the search towards better solutions.

EDAs are typically used in combinatorial optimization problems where the search space is discrete and the goal is to find the best combination of decision variables that optimize a given objective function. The main steps of an EDA include initializing a population of candidate solutions, estimating the probability distribution of promising solutions from the population, sampling new candidate solutions from the estimated distribution, and updating the population with the new solutions.

IMPLICIT AND EXPLICIT MODELS

- Selection, recombination (crossover), and mutation are used to sample the search space

- We may decide to build an explicit model of the space and use it to sample new solutions

- This is an indirect way of performing selection, recombination, and crossover by using an explicit model

  L> BECAUSE NOW WE USE PROBABILITY

- The new solutions will then be used to update our model (repeat as many time as desired)

THIS IS THE IDEA OF MAKING ESTIMATION OF DISTRIBUTION ALGORITHMS

MODEL FITTING BY CLASSIFICATION

- We want to sample new solutions in the "good" areas of the search space

- The idea is to use a **classifier** (e.g., decision trees, SVM, etc) to classify a region of the search space as "good" or "bad" based on the current population

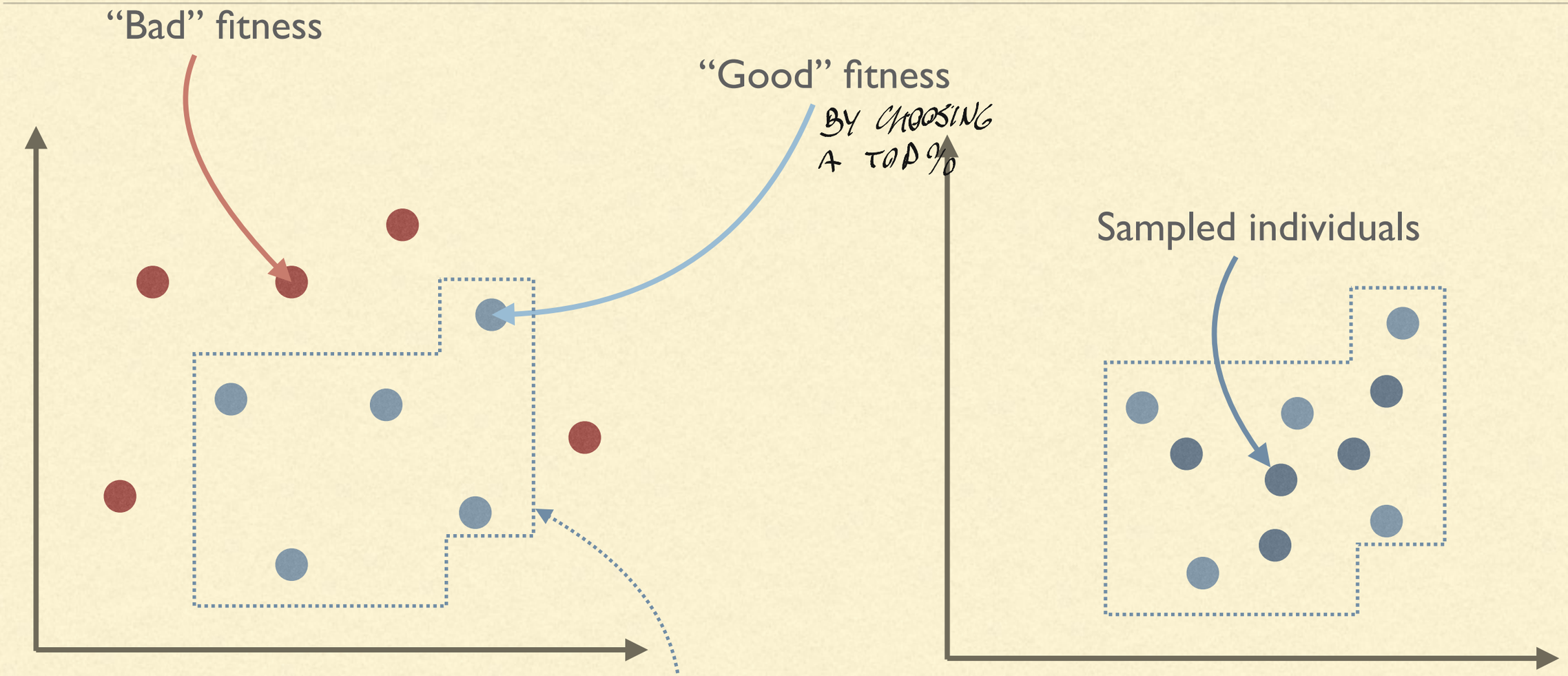
  THE IDEA: IF WE HA A SET SAMPLE WE CAN SPLIT AND CLASSIFY GOOD OR BAD AND ONLY CHOOSE FROM GOOD

- We then use the information provided by the classifier to generate a new population

  ⚠ WE NEED A GOOD CLASSIFIER

- The most famous approach are the **Learnable Evolution Models** (LEM)

CLASSIFICATION



LEARNABLE EVOLUTION MODEL

- Perform some evolutionary steps
- Divide the population in "fit" and "unfit" individuals

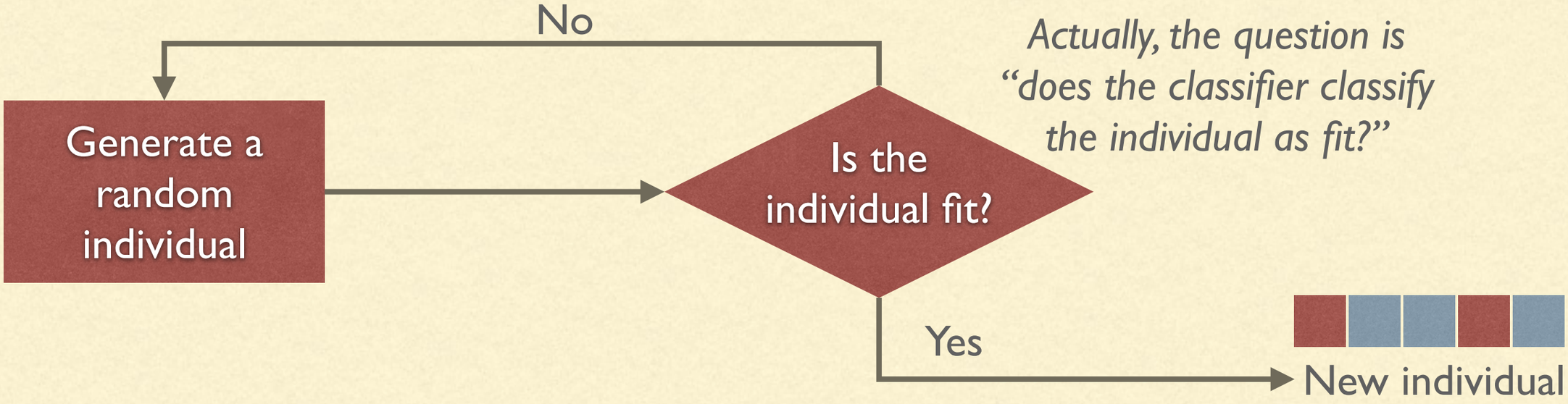
DEPENDS ON THE COMPLEXITY OR THE SAMPLES

- Train a classifier (e.g., SVM, Neural Networks, Decision Trees) to distinguish between fit and unfit individuals
- Remove the unfit individuals and replace them with individuals classified as "fit"
- Go to the first step unless some termination criteria has been met

GENERATIVE VS DISCRIMINATIVE MODELS

- We can divide the models in two classes:
  - **Generative**. They can be used directly to generate new individuals
  - **Discriminative**. Given an individual they can discriminate if the individual is "good" or "bad"
- Classifier are generally discriminative models, hence we usually employ them with *rejection sampling*.

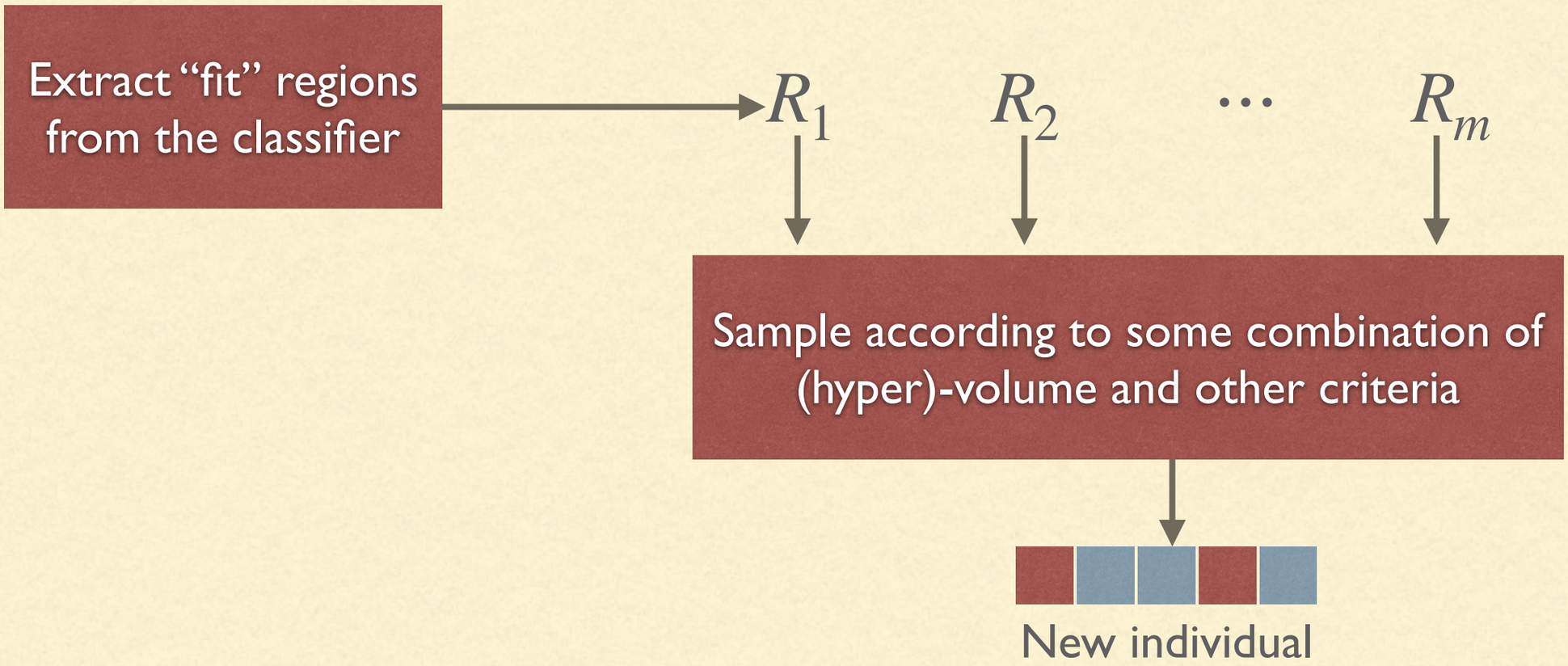
REJECTION SAMPLING



Actually, the question is "does the classifier classify the individual as fit?"

- We can impose a limit on the number of tries (WE HAVE TO)
- After a certain amount of time we have the problem of keeping the number of tries under a reasonable amount
- Most of the search space might be classified as "unfit", so this sampling becomes too expensive
- We can easily extend it to deal with classifications that are not binary (weighted rejection sampling)

REGION-BASED SAMPLING



- Limited only by our ability to extract fit regions from the classifier
- E.g., perfectly possible with decision trees

↳ BUT THEN COMES THE PROBLEMS WITH DECISION TREES

WHAT ARE EDA?

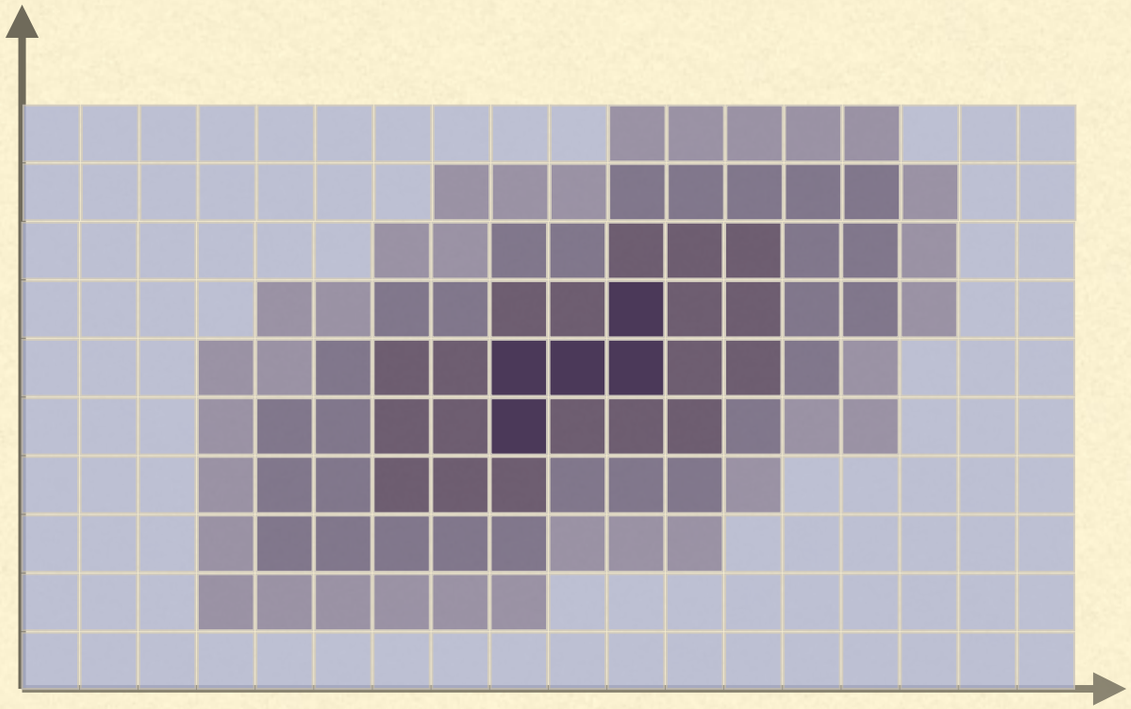
- Sometimes called "probabilistic model-building genetic algorithm" (PMBGA)

- Instead of using an implicit model or a classifier, EDA use directly a probability distribution to sample the new solutions

BECAUSE NOW WE HAVE A SEARCH SPACE (WITH MORE DIMENSION) AND USE P.V. MIGHT BE USEFULL TO FIND MOST PROBABLE GOOD SPACE

HISTOGRAMS

The space can be partitioned into (hyper)cubes and we can compute the average fitness of the samples in each of them



If we split each of the n dimensions in d intervals we have d^n hypercubes

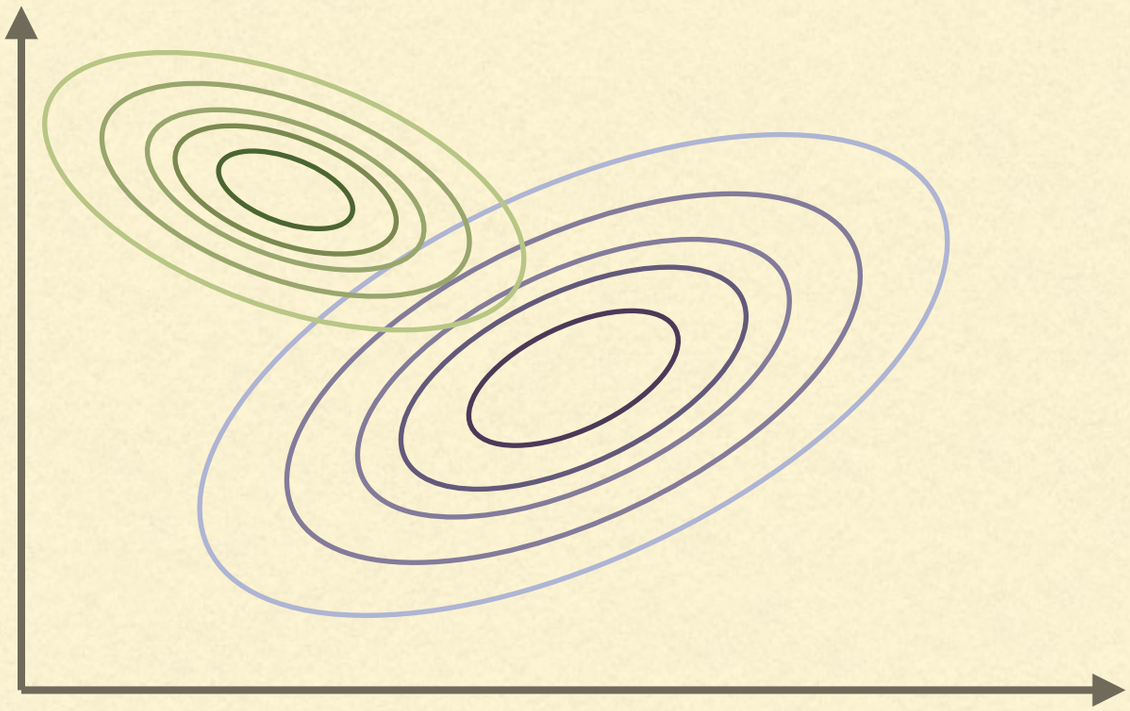
Even for $d = 2$ and a small number of dimensions this is unfeasible

A more compact way of representing the fitness distribution should be used

MULTIPLE GAUSSIAN DISTRIBUTIONS

Instead of representing the distribution as an histogram, we can represent it as the sum of a (fixed) number b of Gaussian distributions in n dimensions

More in general, we can use a collection of "known" distributions and sum them



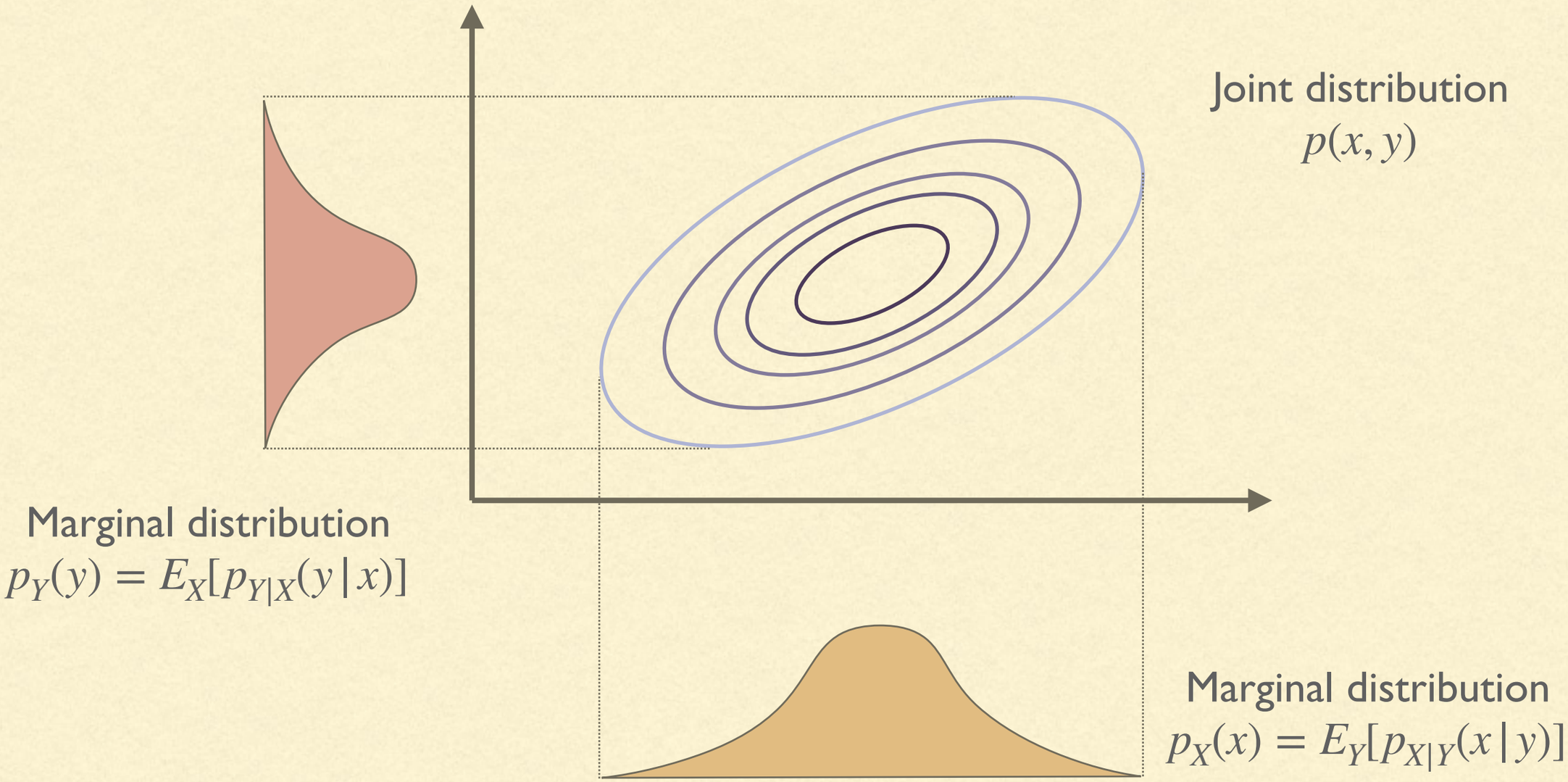
Each Gaussian distribution in n dimensions is determined by:

- The mean vector $\vec{\mu}$ of length n
- The covariance matrix Σ of size n^2

Hence, to represent the distribution as the sum of b Gaussians, we need $b(n + n^2)$ space

THAT IS A MORE REALSTIC STATE SPACE

MARGINAL DISTRIBUTIONS



Joint distribution
$p(x, y)$

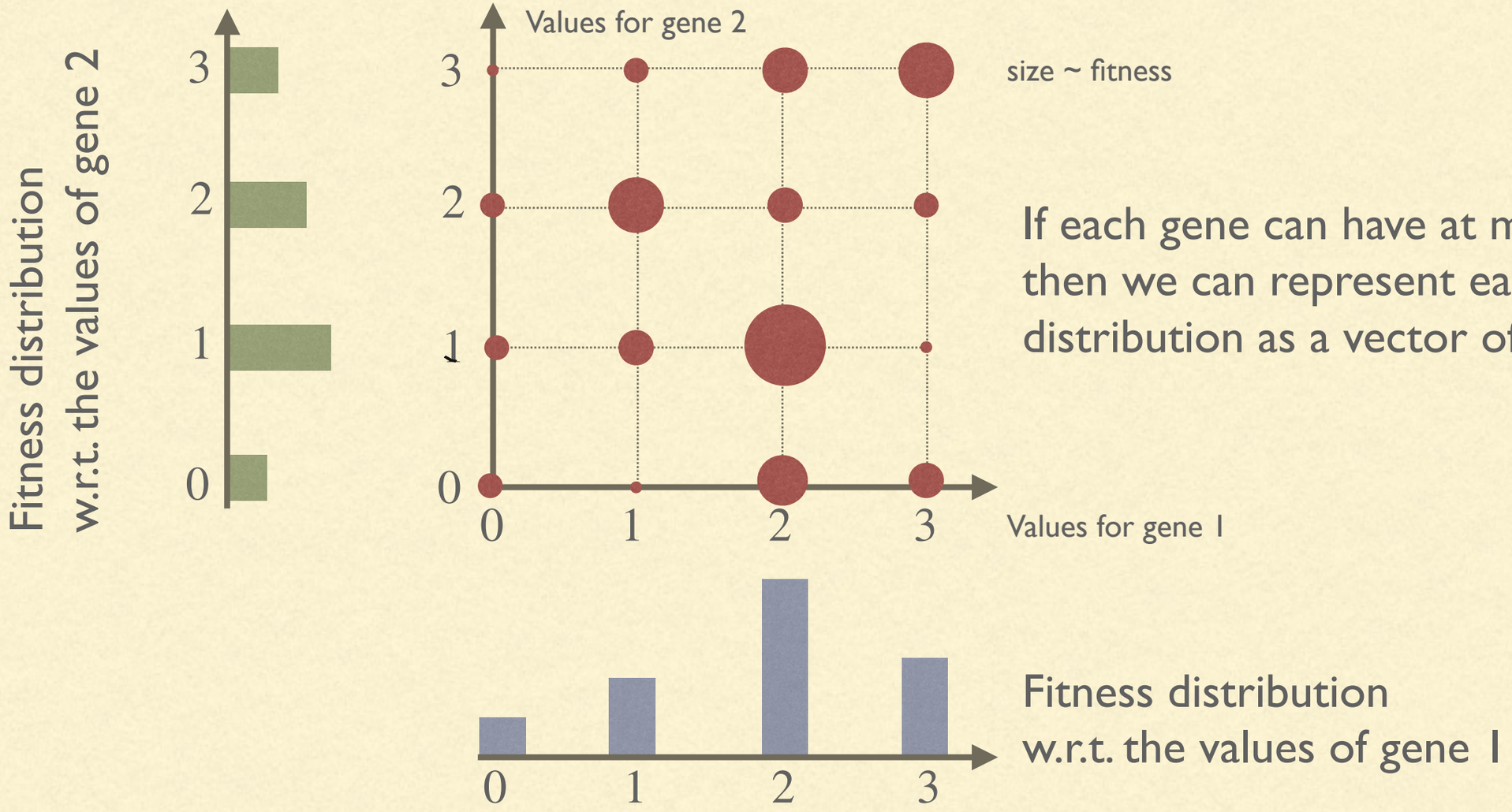
Marginal distribution
$p_Y(y) = E_X[p_{Y|X}(y \mid x)]$

Marginal distribution
$p_X(x) = E_Y[p_{X|Y}(x \mid y)]$

Each (one-dimensional) marginal distribution of b Gaussians requires only a mean and a variance, hence the total space used is $2bn$. BUT YOU ARE LOOSING INFORMATIONS

FINITE DISCRETE SPACES

IN GA WE WORK WITH DISCRETE SPACES



If each gene can have at most k values, then we can represent each marginal distribution as a vector of length $k - 1$

For Boolean spaces we can represent the marginal distributions as a n-dimensional vector with values in $[0,1]$

UNIVARIATE EDA

THIS IS THE SIMPLEST APPROACH (BUT NOT THE EASIEST)

- One standard approach with EDA is to marginalise everything to have only distributions in one dimension
- We are actually assuming that the value of each gene can be determined independently from the values of the others genes

  BUT IT GENERALLY FALSE, STILL FOR SOME PROBLEMS IT MIGHT WORK
- We will see two univariate EDA algorithms:
  - Population-based incremental learning (PBIL)
  - Compact Genetic Algorithm (cGA)

    ↳ EVEN SIMPLYER

POPULATION-BASED INCREMENTAL LEARNING

- For dimension n the algorithm starts with n marginal distributions (initially uniform) $D_1, \ldots, D_n$
- New individuals are sampled picking one gene from each distribution
- Update the marginal distribution according to the fitness of the sampled individuals
- Repeat as needed

PBIL: UPDATE

- Keep the b fittest individuals in the newly sampled population (i.e., truncated selection)

- For each gene j, let N_j be the distribution of values of gene j in the b fittest individuals

- Update $D_j \leftarrow (1-\alpha)D_j + \alpha N_j$ with $\alpha \in [0,1]$

- α allows to change the distribution *gradually*

- ALWAYS ASSUMING THAT WE CONVERGE TO SOMETHING

PBIL: EXTENSIONS

- PBIL can be extended to work in continuous spaces (e.g., $\mathbb{R}^n$)
- One approach is to discrete each marginal distribution into k "buckets"
- Instead of using a discrete distribution we can use a Gaussian for each marginal distribution
- In that case each distribution is defined by μ_{D_j} and $\sigma^2_{D_j}$ and the updating rules must modify them

PBIL: EXTENSIONS

ANOTHER POSSIBILITIE:

- Let P be the current population *after the truncated selection* and $P_{i,j}$ the value of gene j in individual i

- We can compute the following values on P

$$\mu_{N_j} = \frac{1}{|P|} \sum_{P_i \in P} P_{i,j} \qquad \sigma^2_{N_j} = \frac{1}{|P| - 1} \sum_{P_i \in P} (P_{i,j} - \mu_{N_j})^2$$

- And the update of the mean and variance of each marginal distribution is performed as

$$\mu_{D_j} \leftarrow (1 - \alpha)\mu_{D_j} + \alpha\mu_{N_j} \qquad \sigma^2_{D_j} \leftarrow (1 - \beta)\sigma^2_{D_j} + \beta\sigma^2_{N_j}$$

BASICALLY WE ARE ADAPTING μ AND σ^2 BASED ON HOW THE POPULATION CHANGE

COMPACT GENETIC ALGORITHM

- cGA operates *only* over Boolean spaces, WHY?

BECAUSE:

- cGA update the marginal distributions in steps of a fixed size

SO, IT'S EVEN SIMPLER BECAUSE YOU HAVE FIXED SIZE

- Instead of computing a new probability distribution, the individuals in the population are compared in pairs

- For each pair P_i, P_k of individuals, if P_i is fitter than P_k and they differ at gene j, then we shift the distribution D_j to produce the value of gene j in P_i more often

COMPACT GENETIC ALGORITHM

BUT HOW MUCH WE CHANGE DISTRIBUTION ?

- Let $\frac{1}{d}$ be out **discretisation** value (think of it as a "learning rate"). This will be the "step" used to change out distributions

- We identify D_j with the probability of generating a *one* for gene j

- Generate a population P of individuals in which each gene is sampled according to D_j

- For each pair P_i, P_k of individuals, if P_i is fitter than P_k and they differ at gene j, then we shift the distribution D_j to produce the value of gene j in P_i more often (more details later)

Repeat as needed

COMPACT GENETIC ALGORITHM

- For each pair of individuals $P_i, P_k \in P$
  - Let U be the fittest between P_i and P_k and V the other one
  - If $U_j \neq V_j$, $U_j = 0$, and $D_j > 0$
    - $D_j \leftarrow D_j - \frac{1}{d}$ *shift the distribution toward zero*
  - If $U_j \neq V_j$, $U_j = 1$, and $D_j < 1$
    - $D_j \leftarrow D_j + \frac{1}{d}$ *shift the distribution toward one*

FOR EACH GENE WITH DIFFERENT VALUE AND THE BEST IS 0, THEN

WHERE SHIFT JUST MEAN SUBTRACT OR SUM SOME VALUE

SAME WITH 1

ISSUES OF UNIVARIATE EDA

- Univariate EDA assume that the distribution of each gene can be found independently from all the other genes (i.e., no linkage between genes)

- This is usually false (otherwise we would be able to optimise each gene independently)

- Univariate EDA can get stuck in local optima due to this
  WE CAN PROVE TO NOT CONVERGE AT GLOBAL OPTIMA
- **Multivariate EDA** allow to model interaction between genes

BAYESIAN OPTIMISATION ALGORITHM

- Among the different multivariate EDA, one is the Bayesian Optimisation Algorithm (BOA)

- Similar to PBIL where, instead of using marginal distributions, a Bayesian network is used to generate the samples and updated at every generation

- Pelikan, Martin, David E. Goldberg, and Erick Cantú-Paz. *"BOA: The Bayesian optimization algorithm."* Proceedings of the genetic and evolutionary computation conference GECCO-99. Vol. 1. 1999.