stochastics and probability

Lecture 10

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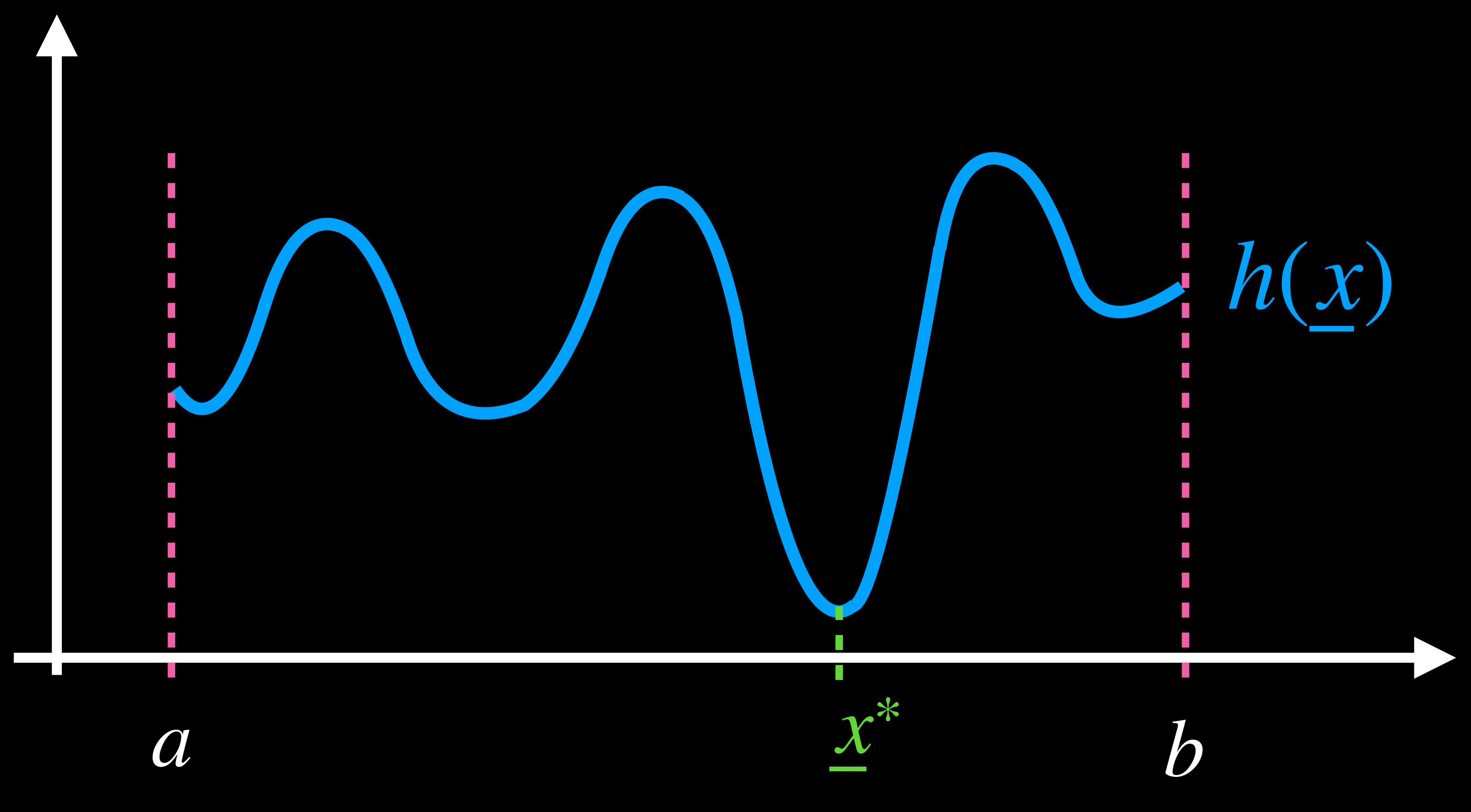
optimization



$\mathbb{S} := [a, b]$

Goal:

$$\underline{x}^* := \underset{\underline{x}\in\mathbb{S}}{\arg\min}\left(h(\underline{x})\right) \qquad \left(\longleftrightarrow \qquad h(\underline{x}^*) = \min_{\underline{x}\in\mathbb{S}}\left(h(\underline{x})\right) \right)$$

Challenges:

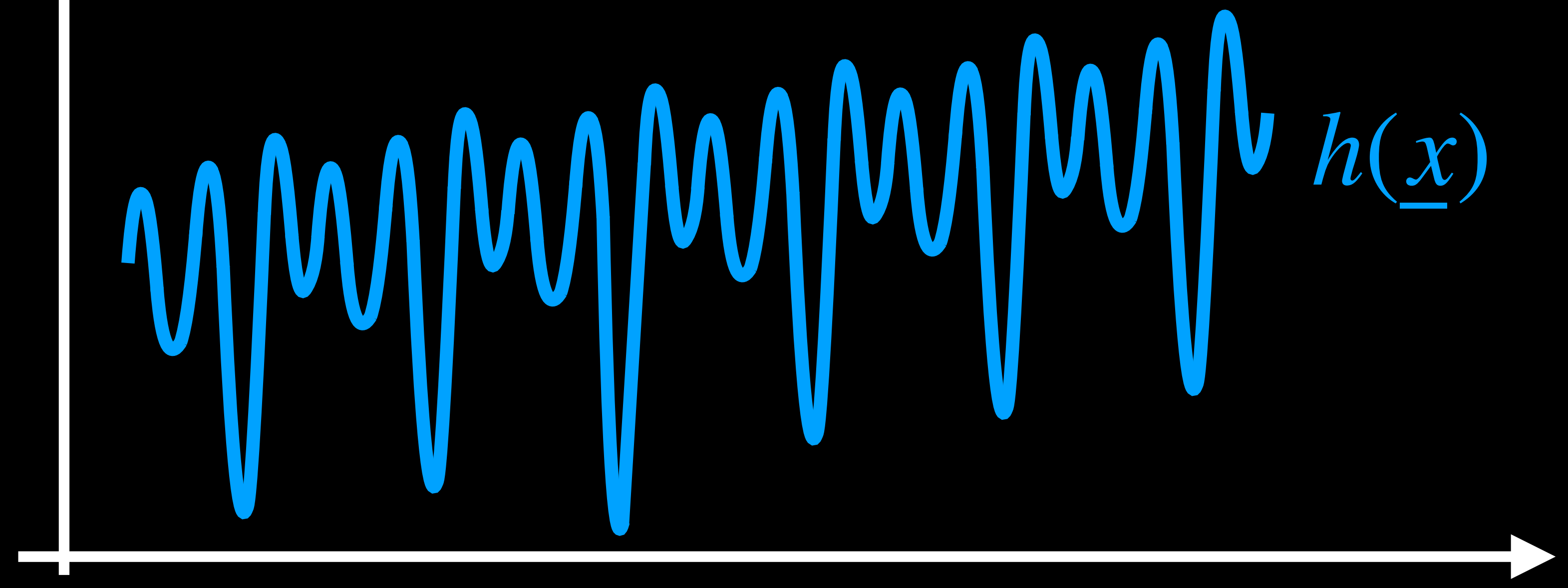
black box

high dimentional

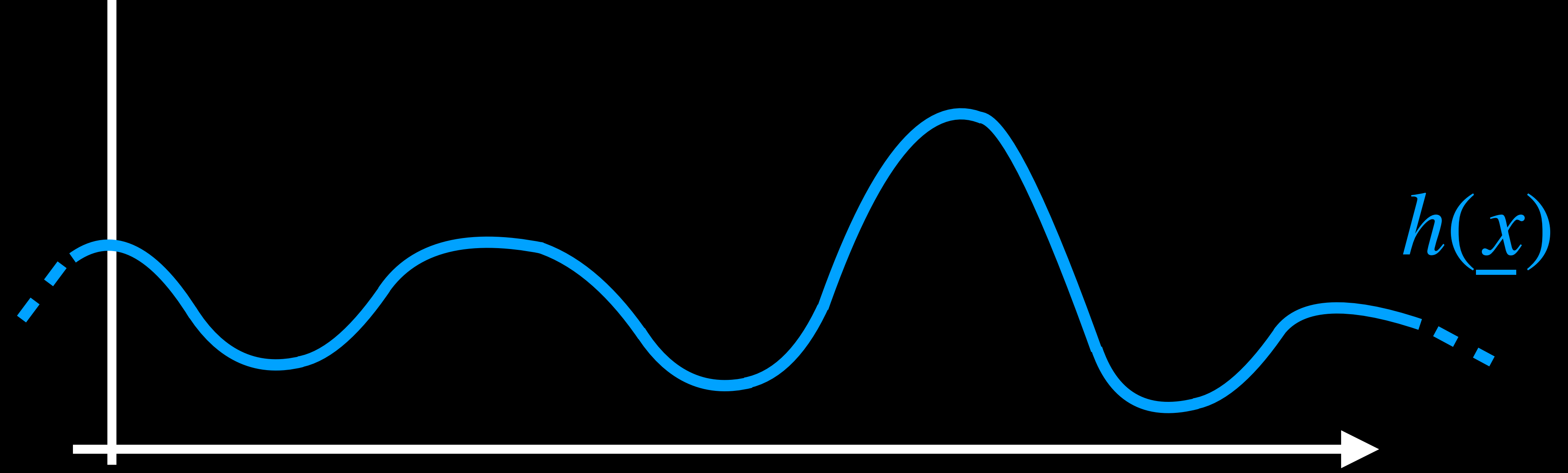
$h(x_1, x_2, x_3, \ldots, x_{100})$

function evaluation are expensive

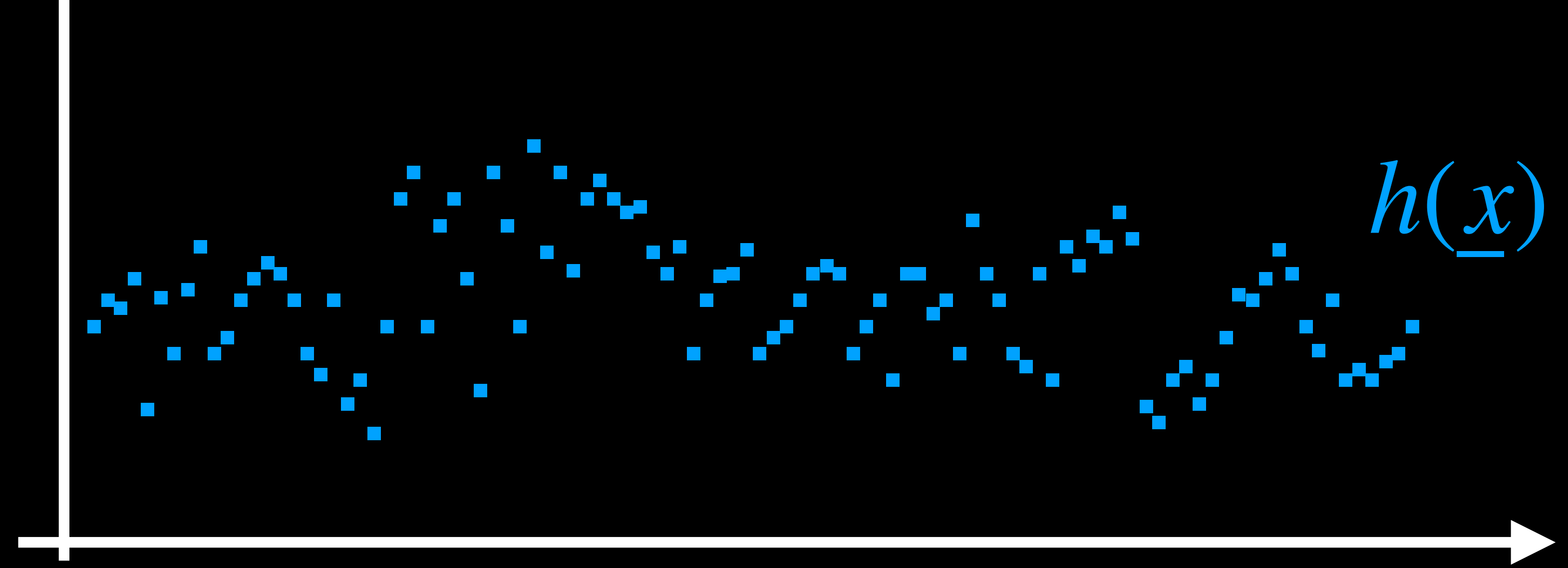
a lot of local minima



infinite support



discrete

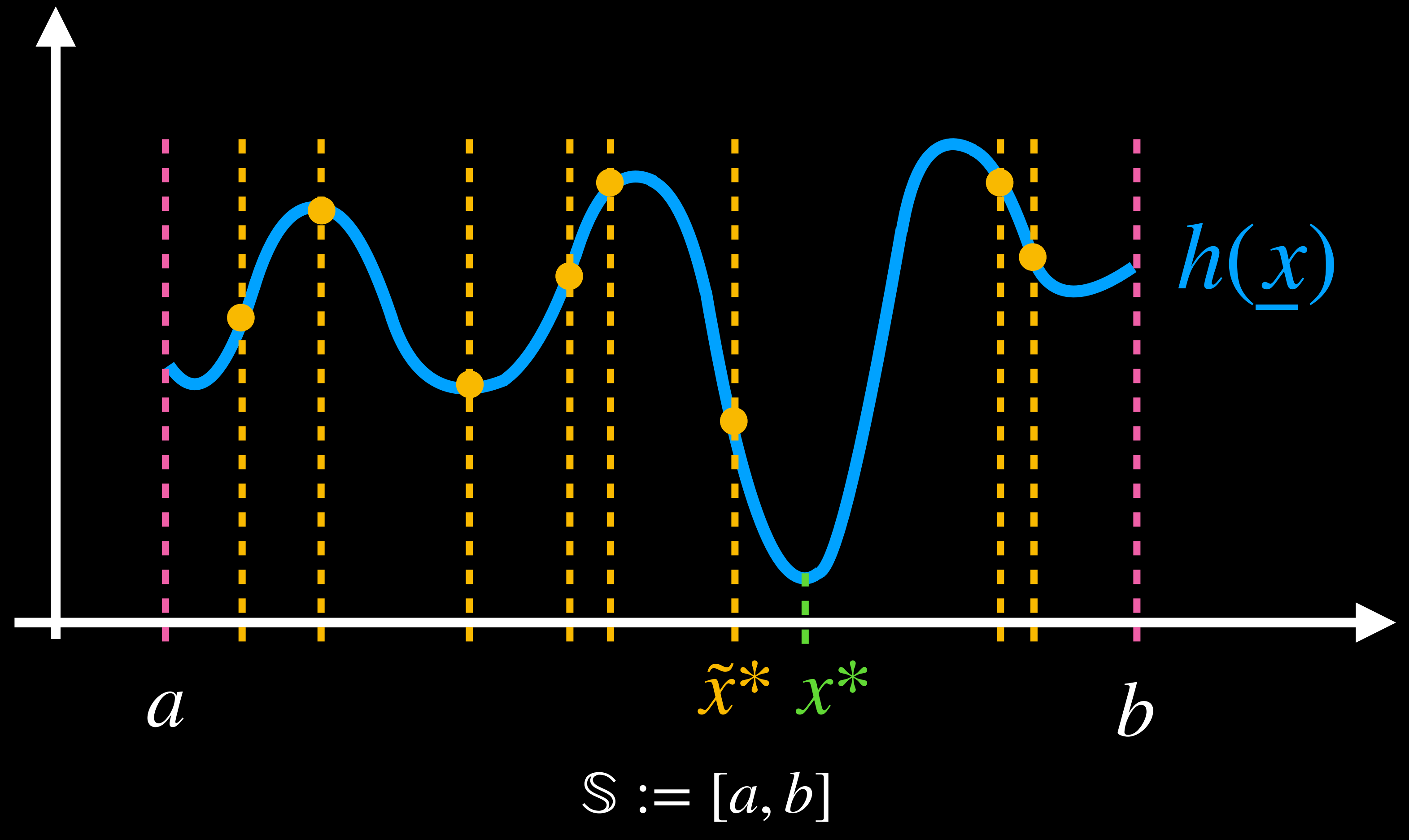


algorithm 1: stochastic exploration

$$\underline{x}^* := \arg\min_{\underline{x}\in\mathbb{S}} \big(h(\underline{x})\big) \approx \arg\min \Big(h(\underline{X}_1),\ldots,h(\underline{X}_n)\Big) =: \tilde{\underline{X}}_n^*$$

$\underline{X}_t : \Omega \to \mathbb{S} \subseteq \mathbb{R}^d$

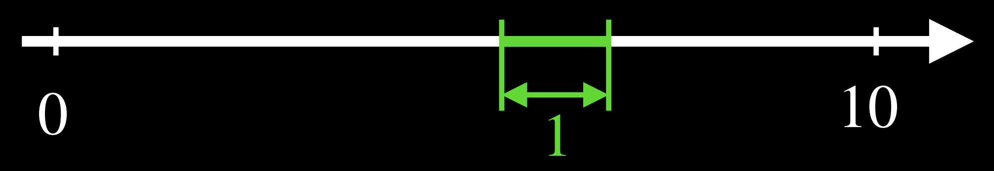
$\underline{X}_t \sim \mathcal{U}(\mathbb{S})$



global convergence:

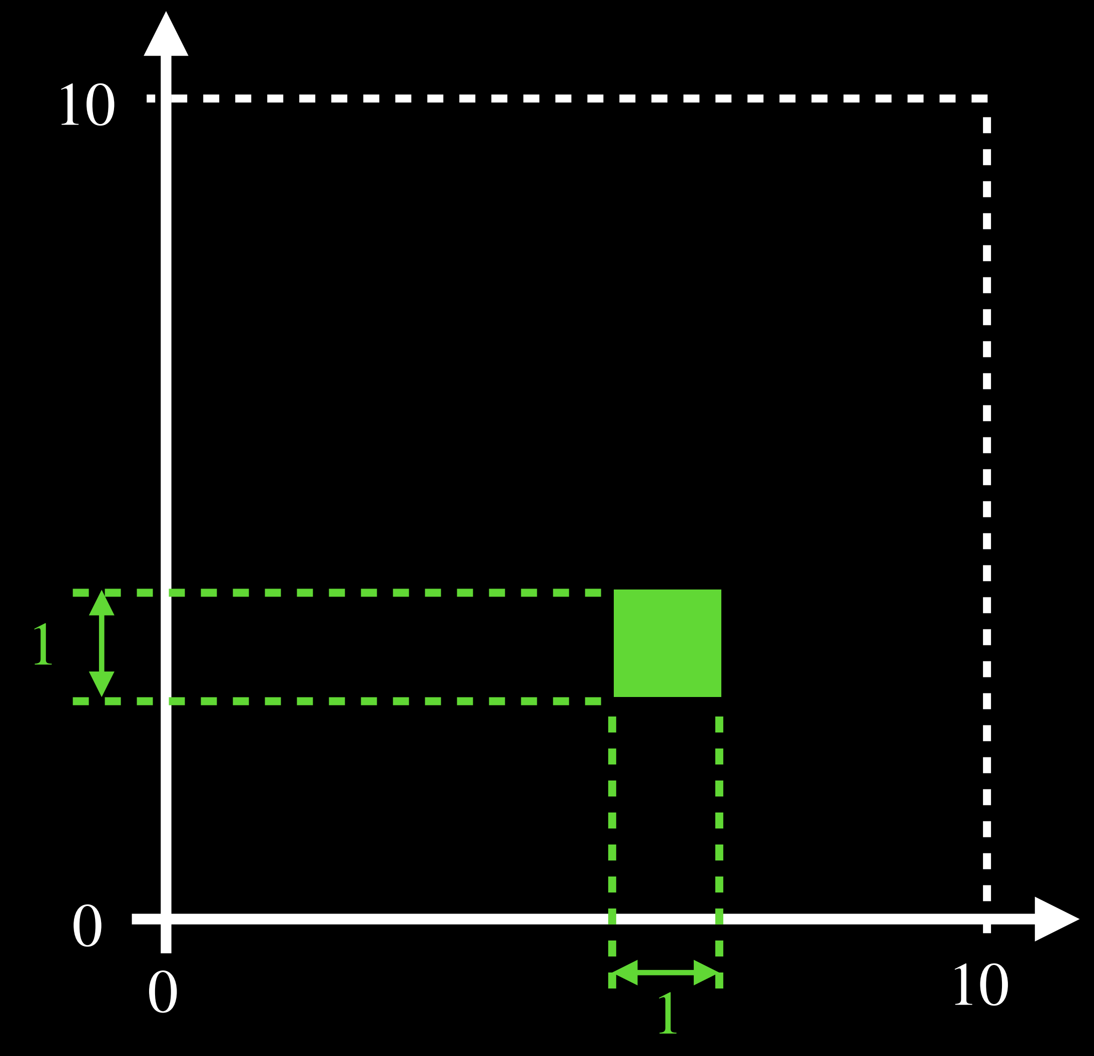
$$\underline{x}^* = \lim_{n\to\infty} \tilde{\underline{X}}_n^*$$

1d:



$P(X \in \text{—}) = \dfrac{1}{10}$

2d:



$P(X \in \blacksquare) = \dfrac{1}{10^2}$

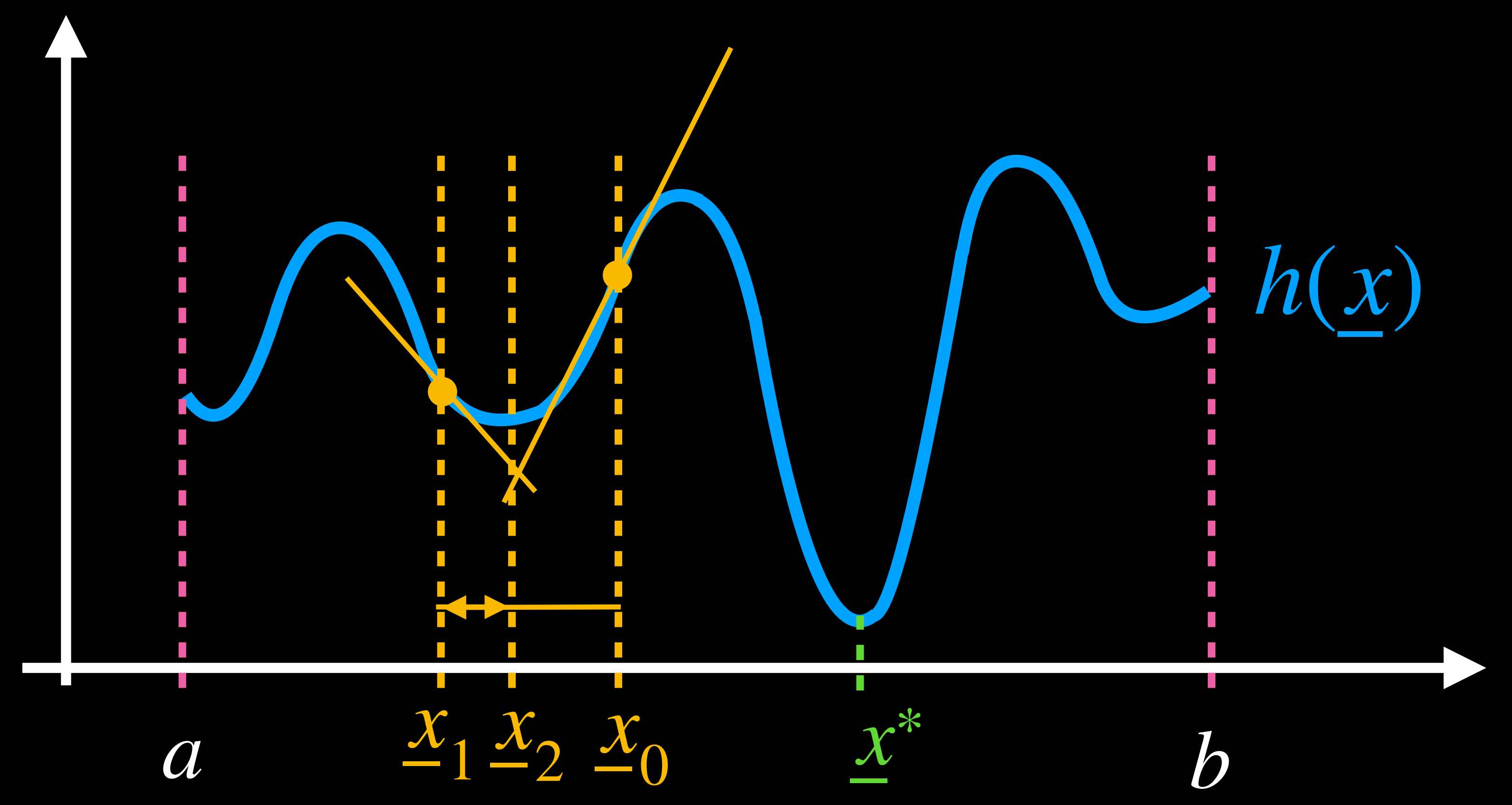
properties:
- very simple
- converges to $\underline{x}^*$

useful if:
- $\mathbb{S}$ is low-dimensional and bounded
- (h is cheap to evaluate for higher dimensions)

$$error \propto n^{-\frac{1}{d}}$$

algorithm 2: stochastic descent

$$\underline{x}^* := \underset{\underline{x}\in\mathbb{S}}{\arg\min}\left(h(\underline{x})\right)$$



gradient descent: $\underline{x}_{t+1} = \underline{x}_t - \alpha_t \boxed{\nabla h(\underline{x}_t)}$

$t \in \{1,\ldots,n\}$	steps
$\alpha_t > 0$	step size
$-\nabla h(\underline{x}_t)$	vector of steepest decrease
$\underline{x}_0$	starting point

gradient:

$$\nabla h(\underline{x}) := \begin{pmatrix} \frac{\partial}{\partial x_1} h(\underline{x}) \\ \vdots \\ \frac{\partial}{\partial x_d} h(\underline{x}) \end{pmatrix}, \qquad \frac{\partial}{\partial x_1} h(\underline{x}) \approx \left(h\begin{pmatrix} x_1 + \Delta x \\ x_2 \\ \vdots \\ x_d \end{pmatrix} - h\begin{pmatrix} x_1 - \Delta x \\ x_2 \\ \vdots \\ x_d \end{pmatrix}\right) \cdot \frac{1}{2\Delta x}$$

→ approximating $\nabla h(\underline{x})$ has $2d$ evaluations of h (expensive)

dot product: $\underline{x} \cdot \underline{y} = \begin{pmatrix} x_1 \\ \vdots \\ x_d \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ \vdots \\ y_d \end{pmatrix} = x_1 y_1 + \ldots + x_d y_d$

stochastic descent:

$$\underline{X}_{t+1} = \underline{X}_t - \frac{\alpha_t}{2\beta_t}\left(\Delta h(\underline{X}_t, \beta_t \underline{U}_t)\right)\underline{U}_t$$

$\underline{U}_t \sim \mathscr{U}(\mathbb{S})$

$\mathbb{S}$ be the d-dimensional unit sphere

β_t sampling radius

directional derivative:

$$\nabla h(\underline{x}) \cdot \frac{\underline{y}}{|\underline{y}|} \approx \frac{\Delta h(\underline{x}, \underline{y})}{2|\underline{y}|}, \qquad \Delta h(\underline{x}, \underline{y}) := h(\underline{x} + \underline{y}) - h(\underline{x} - \underline{y})$$

→ approximation has 2 evaluations of h (cheaper)

properties:

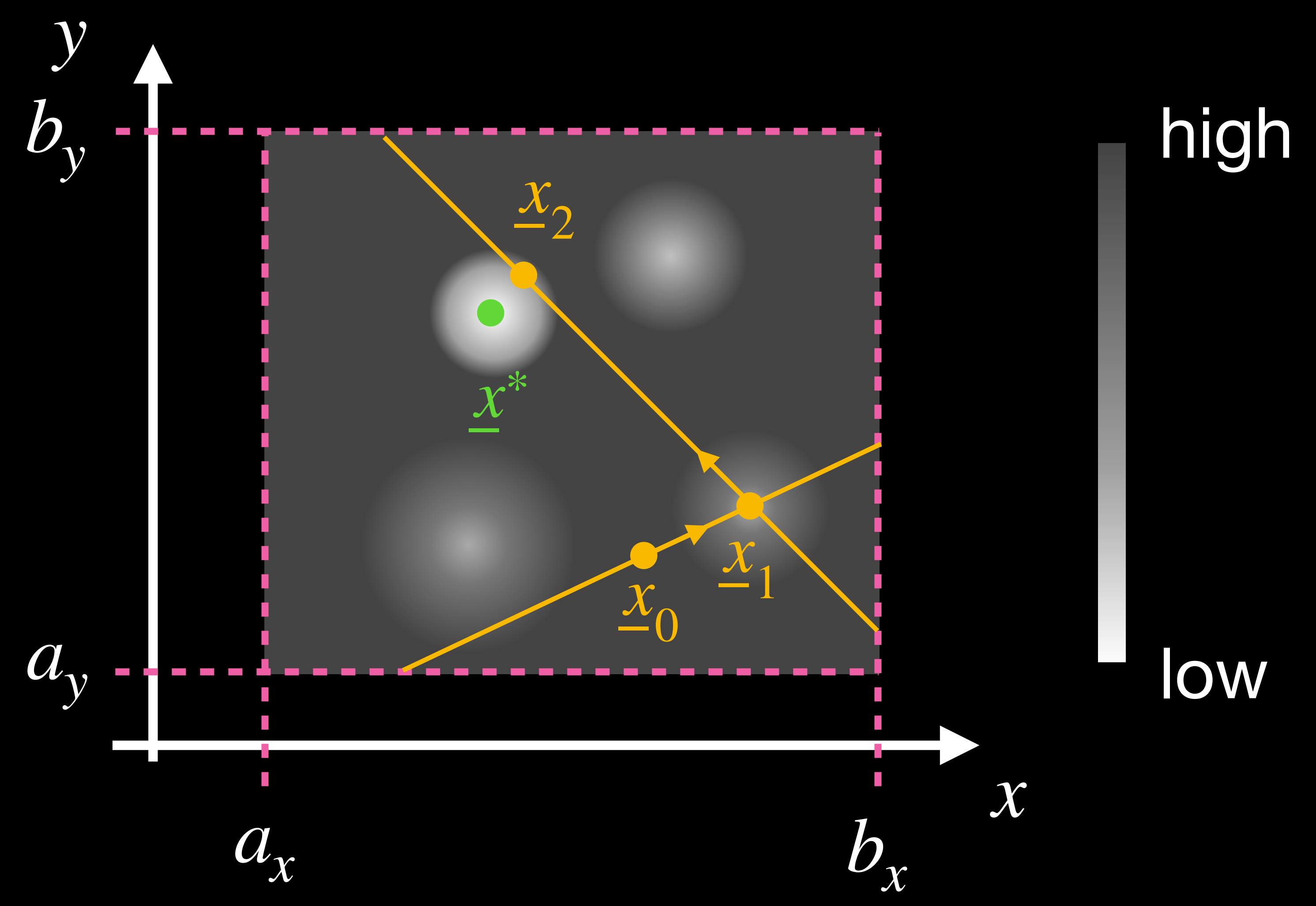
- simple
- no global convergence guarantee
- local convergence if $\lim_{n\to\infty} \alpha_n = 0$ and $\lim_{n\to\infty} \frac{\alpha_n}{\beta_n} = const.$
- converges fast ($\propto \frac{1}{n}$)
- needs uniform random numbers on the unit sphere
- need to choose $\alpha_t, \beta_t, \underline{X}_0$

useful if:

- $\mathbb{S}$ is high-dimensional and unbounded
- h is convex or $\underline{X}_0$ is close to $\underline{x}^*$

algorithm 3: random pursuit

$$\underline{x}^* := \arg\min_{\underline{x}\in\mathbb{S}} \left(h(\underline{x})\right)$$



$$\underline{X}_{t+1} = \underline{X}_t + linesearch(\underline{X}_t, \underline{U}_t) \qquad \underline{U}_t \sim \mathcal{U}(\mathbb{S})$$

$\mathbb{S}$ be the d-dimensional unit sphere

$$linesearch_h(\underline{X}_t, \underline{U}_t) := \arg\min_{\beta} \left(h(\underline{X}_t + \beta \cdot \underline{U}_t)\right) \cdot \underline{U}_t$$

β is distance between X_t and X_{t+1}

(finds the vector to the point with minimal value on the line that goes through $\underline{X}_t$ in the direction $\underline{U}_t$)

$\rightarrow$ reduction to 1d-optimisation problem

properties:

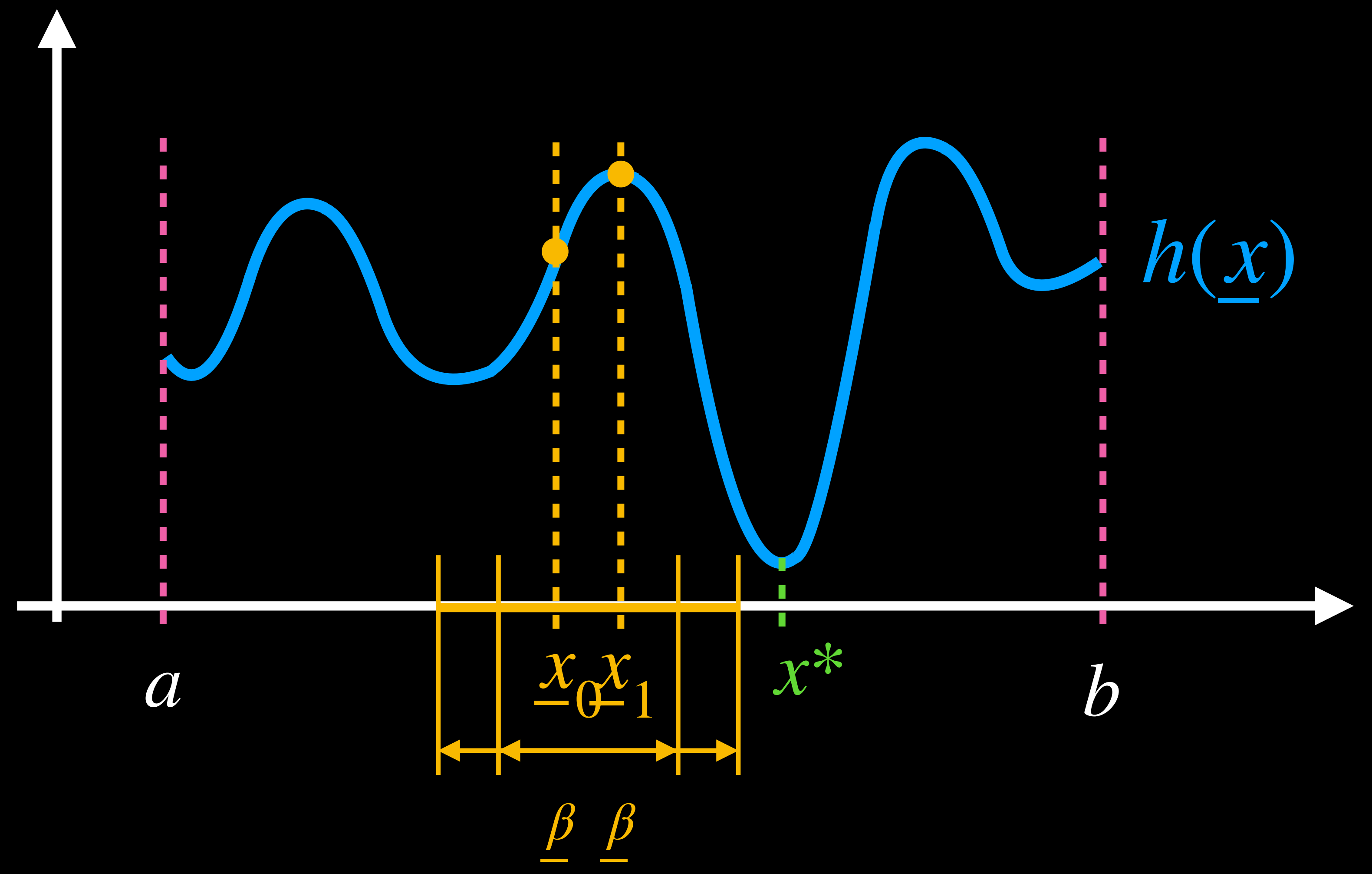
- global convergence guarantee
- converges fast
- needs uniform random numbers (on the unit sphere)

useful if:

- $\mathbb{S}$ is high-dimensional and bounded

algorithm 4: simulated annealing

$$\underline{x}^* := \underset{\underline{x}\in\mathbb{S}}{\arg\min}\,\big(h(\underline{x})\big)$$



$$\underline{X}_{t+1} := \begin{cases} \underline{X}_t + \underline{U}_t^\beta & \text{if } U_t < e^{\frac{h(\underline{X}_t) - h(\underline{X}_t + \underline{U}_t^\beta)}{T_t}} \\ \underline{X}_t & \text{else} \end{cases}$$

$$U_t \sim \mathcal{U}(0,1)$$

$$\underline{U}_t^\beta \sim \mathcal{U}(-\tfrac{1}{2}\underline{\beta}, \tfrac{1}{2}\underline{\beta})$$

$T_t > 0$ is the "temperature" (parameter for the chance to accept worse points)

(example for a cooling scheme: $T_{t+1} := 0.95\, T_t$)

properties:

- simple
- convergence to a local minimum
- global convergence for the "right" cooling scheme
- can go out of local minima again

useful if:

- $\mathbb{S}$ is high-dimensional
- finding the global optimum is more important than finding the exact position of a (local/ global) optimum
- h has a lot of local minima
- h is discrete

algorithm 5: evolutionary algorithms

$$\underline{x}^* := \arg\min_{\underline{x}\in\mathbb{S}} \left(h(\underline{x})\right)$$

$\underline{Y}_t$	child
$\underline{X}_t$	parent
$\underline{N}_t$	mutation
$\mathcal{N}\left(\underline{0},\underline{\underline{\Sigma}}\right)$	multivariate Gaussian
$\underline{\underline{\Sigma}}$	co-variance matrix

(1+1)-ES:

(ES = Evolution Strategy)

$$\underline{Y}_t = \underline{X}_t + \underline{N}_t \qquad \underline{N}_t \sim \mathcal{N}\left(\underline{0},\underline{\underline{\Sigma}}\right)$$

$$\underline{X}_{t+1} = \arg\min\left(h(\underline{Y}_t), h(\underline{X}_t)\right)$$

(1+λ)-ES:

$$\underline{Y}_{t,k} = \underline{X}_t + \underline{N}_{t,k} \qquad \underline{N}_{t,k} \sim \mathcal{N}\left(\underline{0},\underline{\underline{\Sigma}}\right)$$

$$\underline{X}_{t+1} = \arg\min\left(h(\underline{Y}_{t,1}),\ldots,h(\underline{Y}_{t,\lambda}), h(\underline{X}_t)\right)$$

(μ,λ)-ES & (μ+λ)-ES :

recombination

$$\boxed{\left(\underline{Y}'_{t,1},\ldots,\underline{Y}'_{t,\lambda}\right) = recombination\left(\underline{X}_{t,1},\ldots,\underline{X}_{t,\mu}\right)}$$

mutation

$$\boxed{\underline{Y}_{t,k} = \underline{Y}'_{t,k} + \underline{N}_{t,k} \qquad \underline{N}_{t,k} \sim \mathcal{N}\left(\underline{0},\underline{\underline{\Sigma}}\right)}$$

selection

$$\left(\underline{X}_{t+1,1},\ldots,\underline{X}_{t+1,\mu}\right) = selection_{(\mu,\lambda)\text{-ES}}\left(\underline{Y}_{t,1},\ldots,\underline{Y}_{t,\lambda}\right)$$

$$\left(\underline{X}_{t+1,1},\ldots,\underline{X}_{t+1,\mu}\right) = selection_{(\mu+\lambda)\text{-ES}}\left(\underline{Y}_{t,1},\ldots,\underline{Y}_{t,\lambda}, \underline{X}_{t,1},\ldots,\underline{X}_{t,\mu}\right)$$

properties:
- global convergence posible
- (can go out of local minima)

useful if:
- $\mathbb{S}$ is high-dimensional
- finding the global optimum is more important than finding the exact position of a (local/ global) optimum
- h has a lot of local minima
- h is discrete

improvement by
covariance matrix adaptation (CMA)

$$\underline{\underline{\Sigma}}_t$$

- scaling per dimension (different diagonal entries)
- correlations (off-diagonal entries)

end