LECTURE 3: PROBABILISTIC LEARNING AND SAMPLING METHODS

COMPUTATIONAL INTELLIGENCE

VRIJE UNIVERSITEIT AMSTERDAM

PROBABILISTIC LEARNING

TOSS A COIN… 🎶

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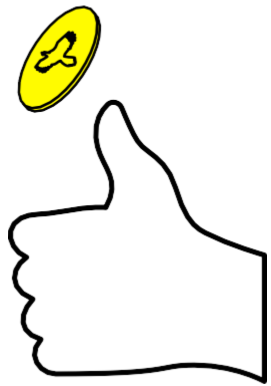

Quick check:

$p(c = 0|x) = x^0 \,(1 - x)^{1-0} = 1 - x$

$p(c = 1|x) = x^1 \,(1 - x)^{1-1} = x$

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EXAMPLE:

$\mathcal{D} = \{0,0,1,1,0,1,1\}$

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- $\mathcal{D} = \{c_1, c_2, \dots, c_N\}$ - *iid* observations (**data**)
- The **likelihood function**:

$$p(\mathcal{D}|x) = \prod_{n=1}^{N} p(c_n|x)$$

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Find such $x \in [0,1]$ that minimizes the **negative log-likelihood function**:

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1) Why **negative**? Because: $\max f(x) = \min \{-f(x)\}$.

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Remarks:

1) Why **negative**? Because: $\max f(x) = \min \{-f(x)\}$.

2) Why **logarithm**? Because: $\log \prod = \sum \log$ and optimum is the same.

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$$\log p(\mathcal{D}|x) = \log \prod_{n=1}^{N} p(c_n|x)$$

the log-likelihood

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$$\log p(\mathcal{D} \mid x) = \log \prod_{n=1}^{N} p(c_n \mid x)$$

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$$= \sum_{n=1}^{N} \log p(c_n \mid x)$$

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$$= \sum_{n=1}^{N} \log x^{c_n} (1 - x)^{1-c_n}$$

Bernoulli distribution

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Bernoulli distribution

$$= \sum_{n=1}^{N} (c_n \log x + (1-c_n) \log(1-x))$$

$\log a^b = b \log a$

$\log ab = \log a + \log b$

TOSS A COIN... 🎶

(Finding $x^\star$) Calculate derivative wrt and set to 0: $\frac{\mathrm{d}}{\mathrm{d}x} f(x) = 0$ gives optimum

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TOSS A COIN... 🎶

(Finding x^*) Calculate derivative wrt   and set to 0:

$$\frac{\mathrm{d}}{\mathrm{d}x} f(x) = 0 \text{ gives optimum}$$

$$\frac{\mathrm{d}}{\mathrm{d}x} \sum_{n=1}^{N} (c_n \log x + (1 - c_n)\log(1 - x)) = 0$$

$$\sum_{n=1}^{N} \left(\frac{c_n}{x} - \frac{(1 - c_n)}{(1 - x)} \right) = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}x} \log x = \frac{1}{x}$$

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$\frac{\mathrm{d}}{\mathrm{d}x} f(x) = 0$ gives optimum

$$\frac{\mathrm{d}}{\mathrm{d}x} \log x = \frac{1}{x}$$

EXAMPLE:

$\mathcal{D} = \{0,0,1,1,0,1,1\}$

$x^\star = 4/7$

PROBABILISTIC LEARNING (LIKELIHOOD-BASED)

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4) Find the best solution by minimizing $-\log p(\mathcal{D}|x)$.

PROBABILISTIC LEARNING (LIKELIHOOD-BASED)

1) Determine $p(y|x)$. — e.g., Bernoulli, Gaussian…

2) Determine $p(\mathcal{D}|x)$. — e.g., *iid* or sequential

3) Check constraints. — e.g., only values between [0, 1]

4) Find the best solution by minimizing $-\log p(\mathcal{D}|x)$. — e.g., using gradient-descent or analytically or DFM

SAMPLING METHODS

HOW TO ESTIMATE π?

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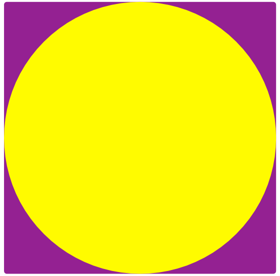
- We know that the circle area is $A_{\bigcirc} = \pi r^2$.
- We know that the square area is $A_{\square} = (2r)^2$.



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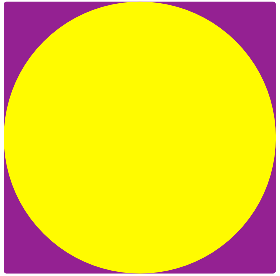

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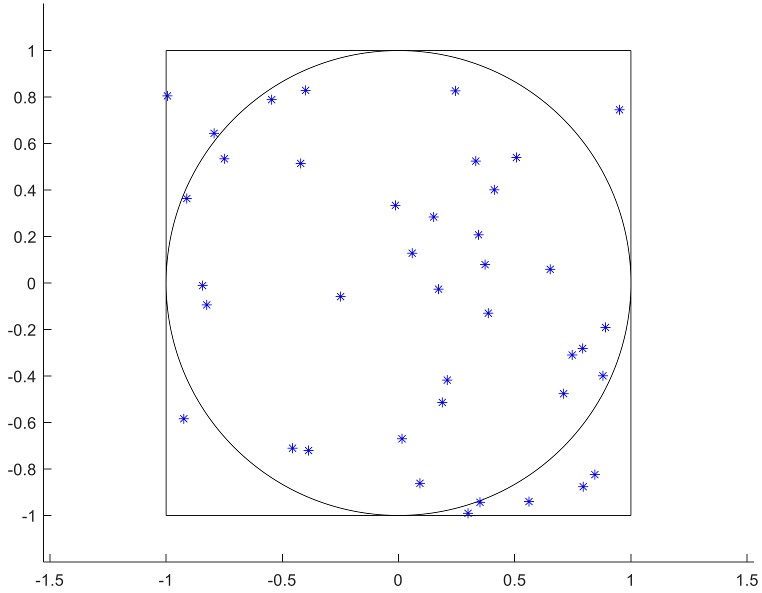

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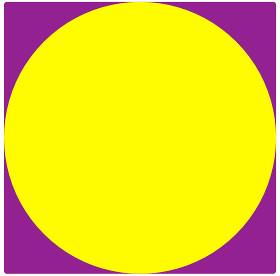

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$$\pi = 4\mathbb{E}_{(x,y)\sim\mathrm{Unif}[-r,r]}\left[\mathrm{I}[x^2 + y^2 \leq r^2]\right]$$

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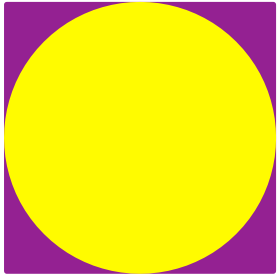
$$\approx 4\frac{1}{N}\sum_{n=1}^{N}\mathrm{I}[x_n^2 + y_n^2 \le r^2]$$



Approximate it by sampling!

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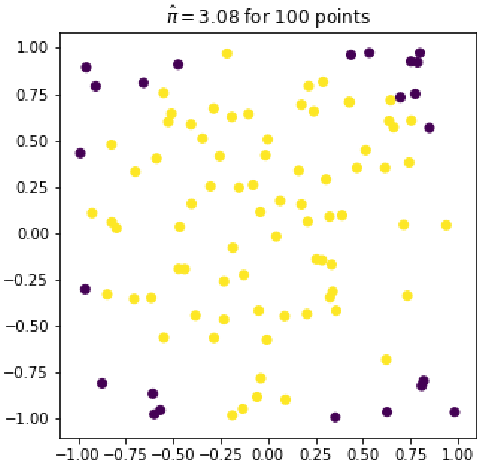

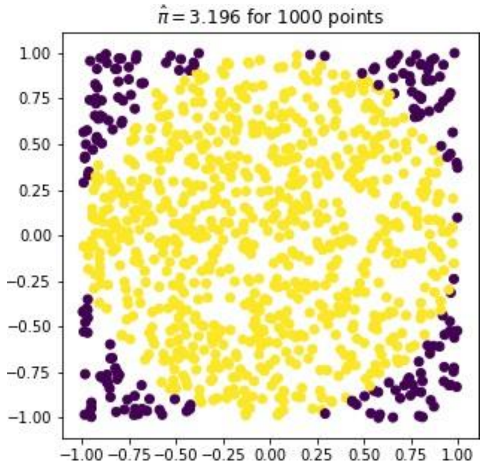

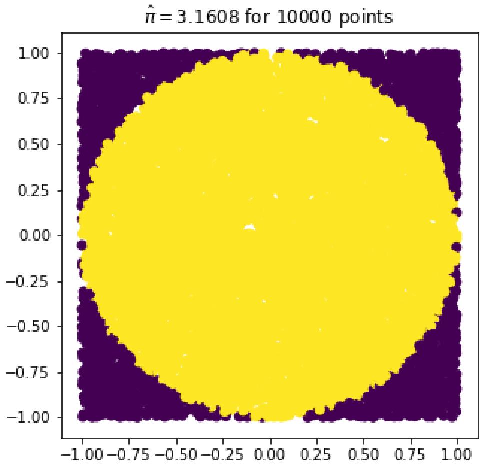

MONTE CARLO METHODS

- History: **Stanisław Ulam** played solitaire and asked himself what are the chances that a particular laid out with 52 cards is successful.

Stanisław Ulam (1909-1984) was a Polish mathematician, a participant of the Manhattan project, known for applications of mathematics to physics, biology and computer science, and first formulations of Monte Carlo methods and cellular automata (with John von Neumann).

MONTE CARLO METHODS

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- The underlying idea: **Approximate by sampling**!

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- General applications:

  A. **Analytically infeasible quantities** (e.g., normalization constants, statistical inference, expectations of some function of interest).

  B. **Optimization**.

MONTE CARLO METHODS

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And in 10D ➞ 10^{20} points.

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- A natural question is:

Can we do better than independent sampling?

MARKOV CHAIN MONTE CARLO

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- Could any distribution be used as a proposal distribution?

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- In other words, we introduce a **proposal distribution** $q(x_t | x_{t-1})$ to obtain a **chain** that corresponds to a sample from the original distribution $p(x)$.
- Could any distribution be used as a proposal distribution? **NO**.
- Conditions on the proposal distribution:

  A. (**Irreducibility**) There is a positive probability of visiting all states.

  B. (**Aperiodicity**) The chain should not get trapped in cycles.

METROPOLIS-HASTINGS ALGORITHM

1. Initialize $x_t := x_0$.
2. For $t \in \{0,1,\ldots,T-1\}$:

   (i) (**Generate**) Sample $x' \sim q(x|x_t)$.

   (ii) (**Evaluate**) Calculate acceptance probability:

$$A(x', x_t) = \min\left\{1, \frac{p(x')\, q(x_t|x')}{p(x_t)\, q(x'|x_t)}\right\}$$

   (iii) (**Select**) Sample $u \sim \mathrm{Unif}[0,1]$.

   If $A(x', x_t) > u$, then $x_{t+1} := x'$.

   Else $x_{t+1} := x_t$.

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   (i) (**Generate**) Sample $x' \sim q(x|x_t)$. #e.g. $q(x|x_t) = \mathcal{N}(x|x_t, \sigma^2)$
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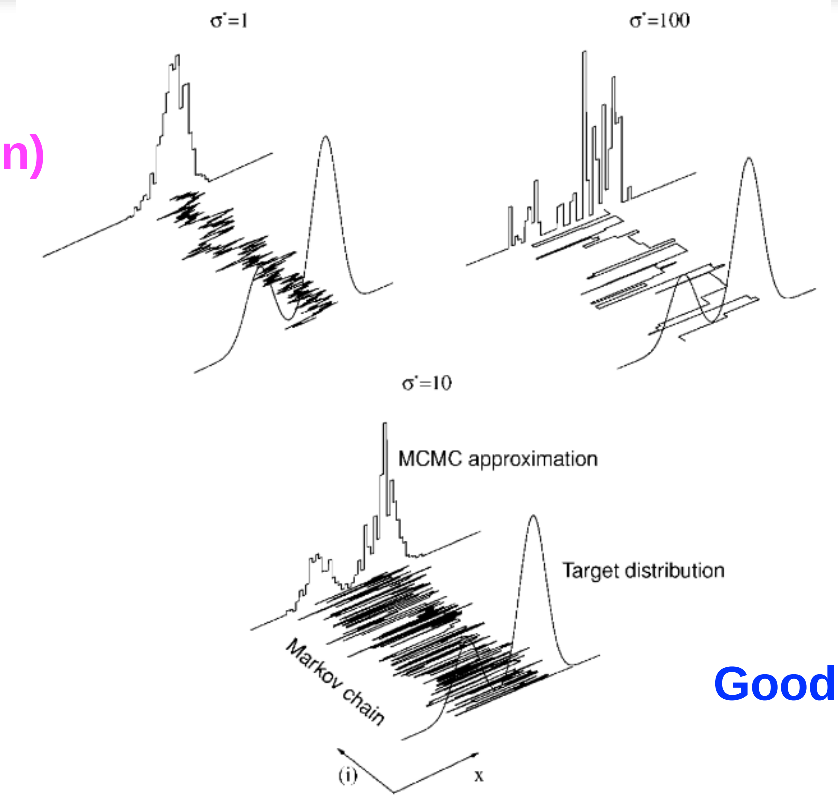
$$\boxed{p(x) \propto \exp(-f(x))}$$

METROPOLIS-HASTINGS ALGORITHM

Too small
(mode omission)



Too large
(low acceptance)

Good!

INDEPENDENT SAMPLER

1. Initialize $x_t := x_0$.
2. For $t \in \{0,1,\dots,T-1\}$:
   (i) (**Generate**) Sample $x' \sim q(x)$.
   (ii) (**Evaluate**) Calculate acceptance probability:

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METROPOLIS ALGORITHM

1. Initialize $x_t := x_0$.
2. For $t \in \{0, 1, \ldots, T-1\}$:
   (i) (**Generate**) Sample $x' \sim q(x|x_t)$, where $q(x'|x_t) = q(x_t|x')$.
   (ii) (**Evaluate**) Calculate acceptance probability:
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SIMULATED ANNEALING

1. Initialize $x_t := x_0$ and $T_t := T_0$.
2. For $t \in \{0, 1, \ldots, T - 1\}$:
   (i) (**Generate**) Sample $x' \sim q(x|x_t)$.
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$$A(x', x_t) = \min\left\{1, \frac{p^{\frac{1}{T_t}}(x')\, q(x_t|x')}{p^{\frac{1}{T_t}}(x_t)\, q(x'|x_t)}\right\}$$

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   If $A(x', x_t) > u$, then $x_{t+1} := x'$.
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   (iv) Set T_{t+1} according to chosen cooling schedule.

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If $p(x) \propto \exp(-f(x))$,
then $p^{\frac{1}{T}}(x) \propto \exp\left(-\frac{1}{T} f(x)\right)$.

SIMULATED ANNEALING

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$$T = C \ln(t + T_0))^{-1}$$

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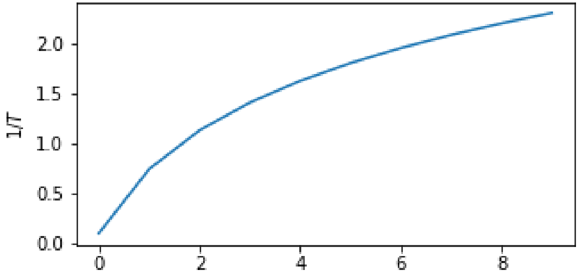


OPTIMIZATION THROUGH SAMPLING

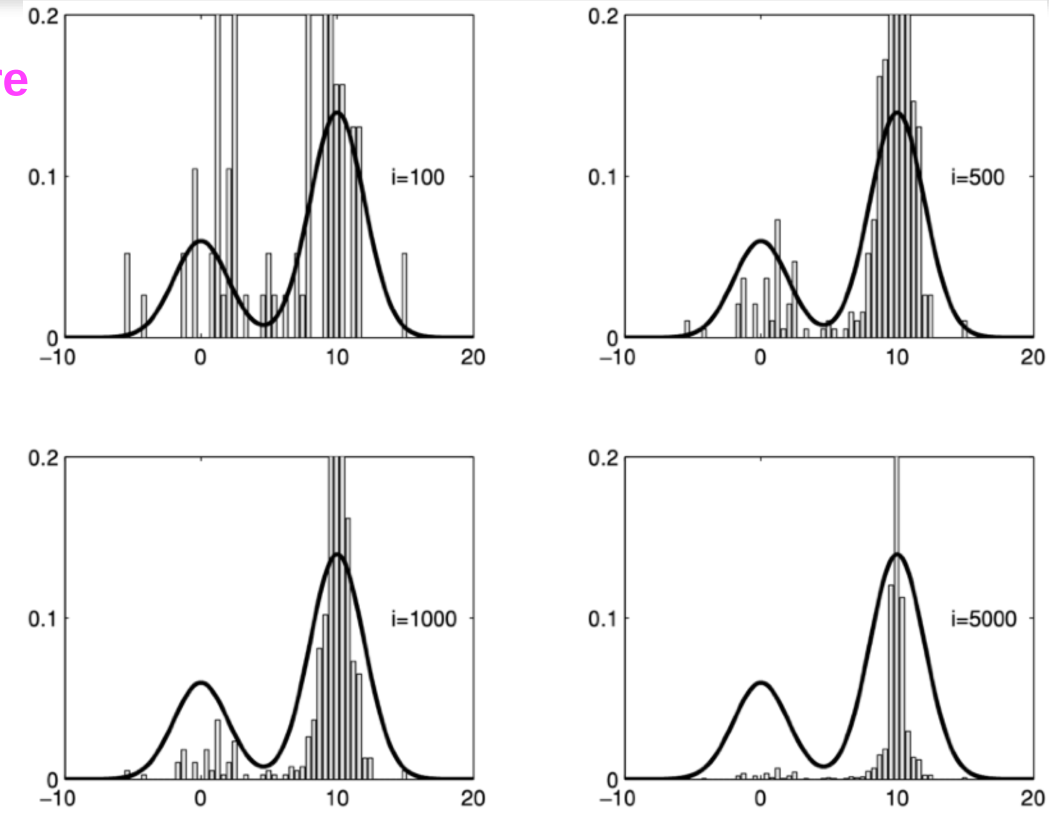
- We are interested in minimizing $f(x)$.
- Alternatively, we can consider a distribution of the form

$$p(x) \propto \exp(-f(x)/T)$$

- By changing the temperature, we can consider almost uniform distribution (high temperature) or peaky distribution (low temperature).
- For uniform distribution we have **exploration**, while for more peaky distribution we have **exploitation**.

EXAMPLE (SIMULATED ANNEALING)

High temperature



Low temperature

METROPOLIS-HASTINGS ALG. VS LOCAL SEARCH

Stochastic search

1. Initialize $x_t := x_0$.
2. For $t \in \{0, 1, \dots, T-1\}$:
   (i) (**Generate**) Sample $x' \sim q(x|x_t)$.
   (ii)(**Evaluate**) Calculate acceptance probability:

$$A(x', x_t) = \min\left\{1, \frac{p(x')\, q(x_t|x')}{p(x_t)\, q(x'|x_t)}\right\}$$

   (iii) (**Select**) Sample $u \sim \mathrm{Unif}[0,1]$.
   If $A(x', x_t) > u$, then $x_{t+1} := x'$.
   Else $x_{t+1} := x_t$.

Deterministic search

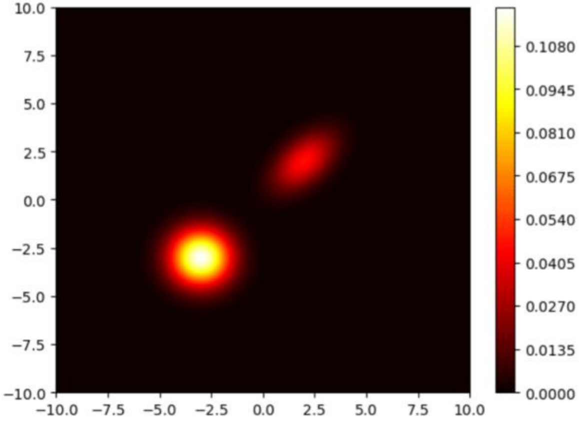
1. Initialize a solution.
2. For $t \in \{0, 1, \dots, T-1\}$:
   (i)(**Generate**) Generate solutions in the neighborhood of the current best solution.
   (ii)(**Evaluate**) Evaluate the potential solutions.
   (iii)(**Select**) Pick the solution with best objective as the best current solution.

ASSIGNMENT 2: Sampling

The goal is to implement Metropolis-Hastings (MH) and Simulated Annealing (SA) algorithms and analyze their behavior.
Here, we are interested in sampling from a mixture of two Gaussians, namely:

Target distribution: $p(\mathbf{x}) = 0.25 \cdot \mathcal{N}\left(\mu = \begin{bmatrix} 2 \\ 2 \end{bmatrix}, \Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}\right) + 0.75 \cdot \mathcal{N}\left(\mu = \begin{bmatrix} -3 \\ -3 \end{bmatrix}, \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right)$

Visualization:



Thank you!

VU VRIJE UNIVERSITEIT AMSTERDAM

EXTRA READING

Andrieu et al., "An Introduction to MCMC for Machine Learning", Machine Learning, Vol. 50, pp. 5-43, 2003

Ch. Bishop, "Pattern Recognition and Machine Learning", Springer

K. Murphy, "Machine Learning: A Probabilistic Perspective", The MIT Press