Monte Carlo Markov Chain

Bayesian methods

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Most of the material in this presentation is taken from

“**Information Theory, Inference, and Learning Algorithms**”

by **David J. C. McKay**.

Free pdf at https://www.inference.org.uk/itprnn/book.pdf

Suggested reading: “Handbook of Markov chain Monte Carlo” by S. Brooks, A. Gelman, G. L. Jones and X.-L. Meng

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Recap of the Bayes' theorem

$$P(x\,|\,y) = \frac{p(y\,|\,x)p(x)}{p(y)}$$

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This is also a conditional probability. This is the probability of y given that x is true; it can also be interpreted as the **Likelihood** of x given y

This is the probability of observing x without further condition. It is also known as the **prior probability**.

This is the probability of y without any given conditions; this is known as the **evidence**. It can be written as: $P(y) = \int p(y|x)p(x)dx$

Monte Carlo methods

The goal

Monte Carlo methods are computational techniques that make use of random numbers. The aims of MC methods is to solve one or both of the following problems:

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Monte Carlo methods are computational techniques that make use of random numbers. The aims of MC methods is to solve one or both of the following problems:

- Generate samples $\{\mathbf{x}_\mathrm{i}\}_{\mathrm{i}=1}^{\mathrm{N}}$ from a probability distribution $P(\mathbf{x})$
- Generate expectation of functions under this distribution. For instance:

$$\Phi = \langle \phi(\mathbf{x}) \rangle = \int d^N P(\mathbf{x}) \phi(\mathbf{x})$$

Monte Carlo methods

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Some examples of $\phi(\mathbf{x})$ can be the first order moments of the target density, i.e. mean and variance.

So let's assume that $P(\mathbf{x})$ is too complicated and its moments can't be evaluated in some exact way. **We want to use Monte Carlo methods**.

Monte Carlo methods

The sampling problem

- Let's focus on the **sampling problem**, because if we solve this, then generating the expectation function is straightforward using the random samples $\{\mathbf{x}^{(\mathrm{i})}\}_{\mathrm{i}=1}^{\mathrm{N}}$ to build the estimator:

$$\hat{\Phi} = \frac{1}{N} \sum \phi_i(\mathbf{x})$$

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- The estimator is unbiased as long as $\{\mathbf{x}^{(\mathrm{i})}\}_{\mathrm{i}=1}^{\mathrm{N}} \sim P(\mathbf{x})$.

Monte Carlo methods

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Property of MC methods: The accuracy of an MC estimate depends only on the variance of ϕ, not on the parameter space dimension. Precisely, the variance of $\hat{\Phi}$ decreases with the number of samples.

- However, sampling from high-dimensionality can be a problem in MC methods; drawing samples from $P(\mathbf{x})$ is not easy in general.

Monte Carlo methods

The sampling problem

- Let’s assume we can evaluate $P(\mathbf{x})$ up to a normalization constant, i.e. we can evaluate $P^*(\mathbf{x}) = P(\mathbf{x})/Z$.

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  A. We do not know the normalization constant $Z = \int P^*(\mathbf{x}) d^N \mathbf{x}$, and

  B. Even if we knew Z, it would still be challenging to sample in a high-dimensional space without exploring most of all the possible states.

Monte Carlo methods

The sampling problem

- To draw samples from $P(\mathbf{x})$ we need to explore the space where $P(\mathbf{x})$ is large, and we can only guess where it happens by evaluating the density *everywhere*.

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Monte Carlo methods

The sampling problem

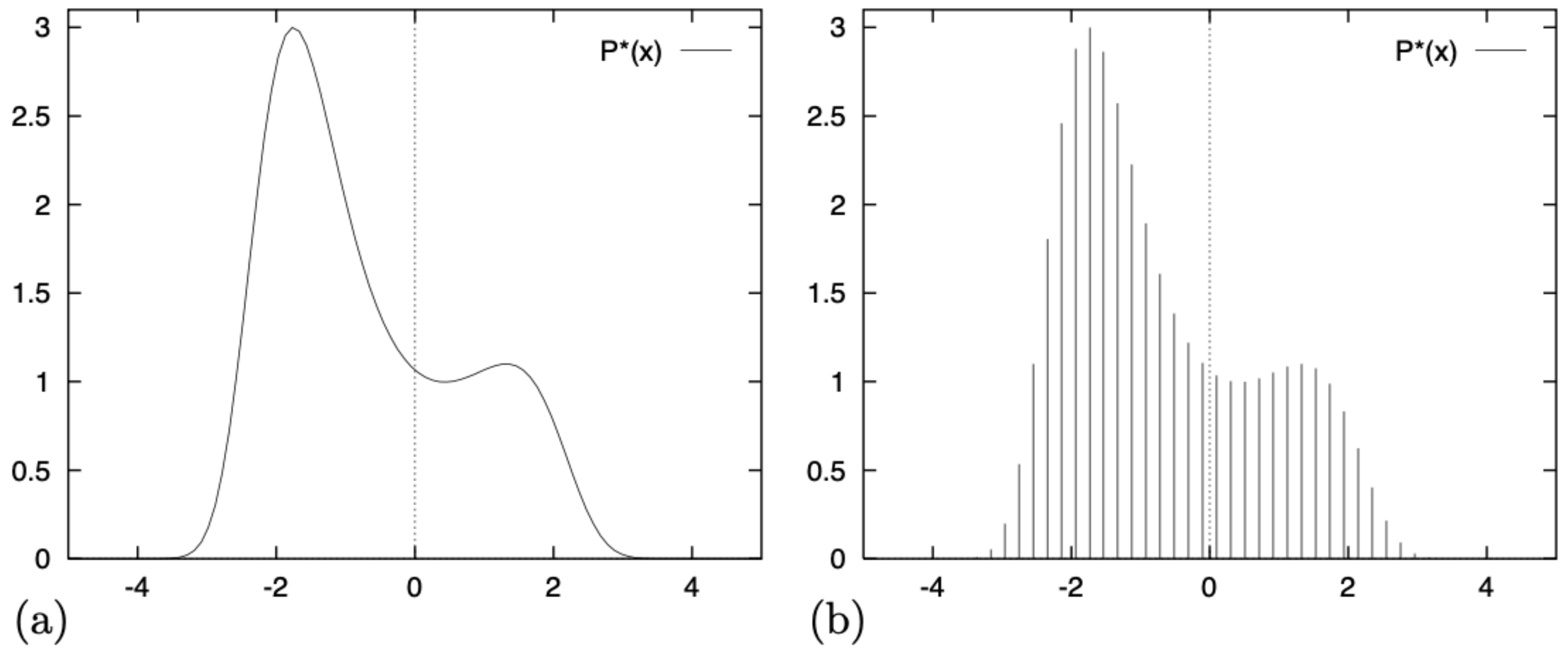
- To draw samples from $P(\mathbf{x})$ we need to explore the space where $P(\mathbf{x})$ is large, and we can only guess where it happens by evaluating the density *everywhere*.
- We know a convenient way to draw samples from very few distributions; the Normal distribution is of course one of these.

Monte Carlo methods

A simple 1D example

- We want to draw samples from $P^*(x) = P(x)/Z$, with:

$$P^*(x) = e^{0.4(x-0.4)^2 - 0.08x^4}$$



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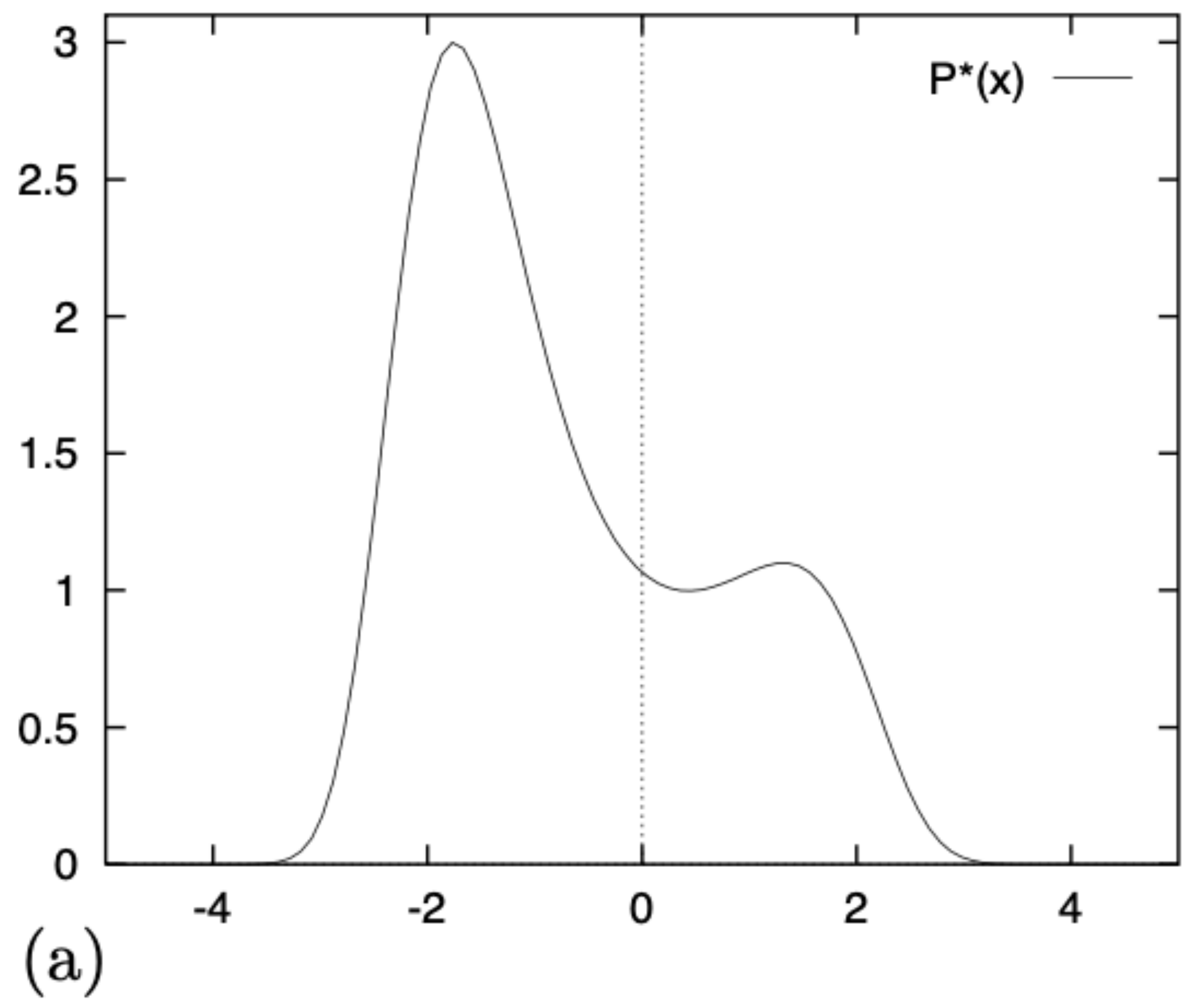

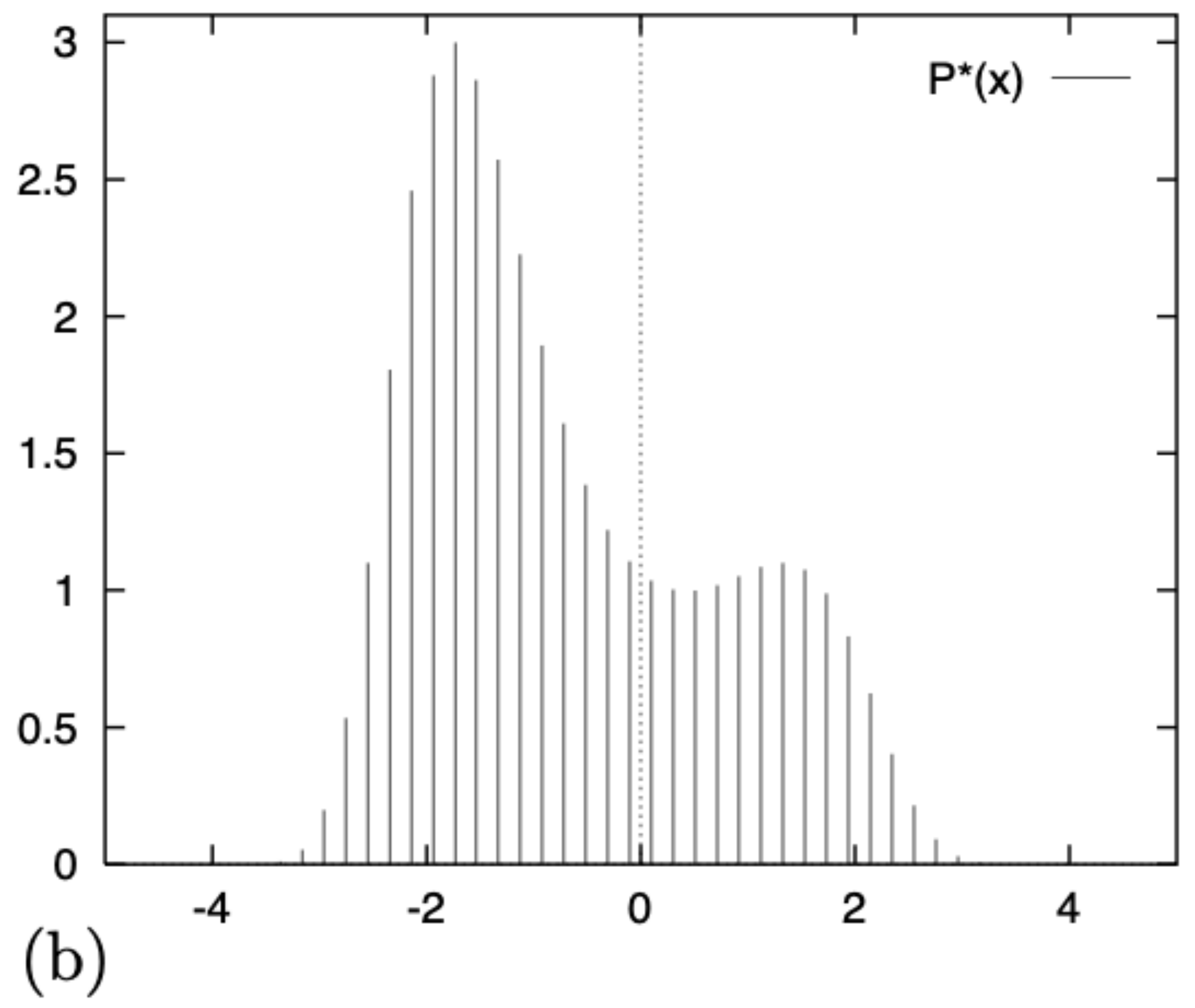

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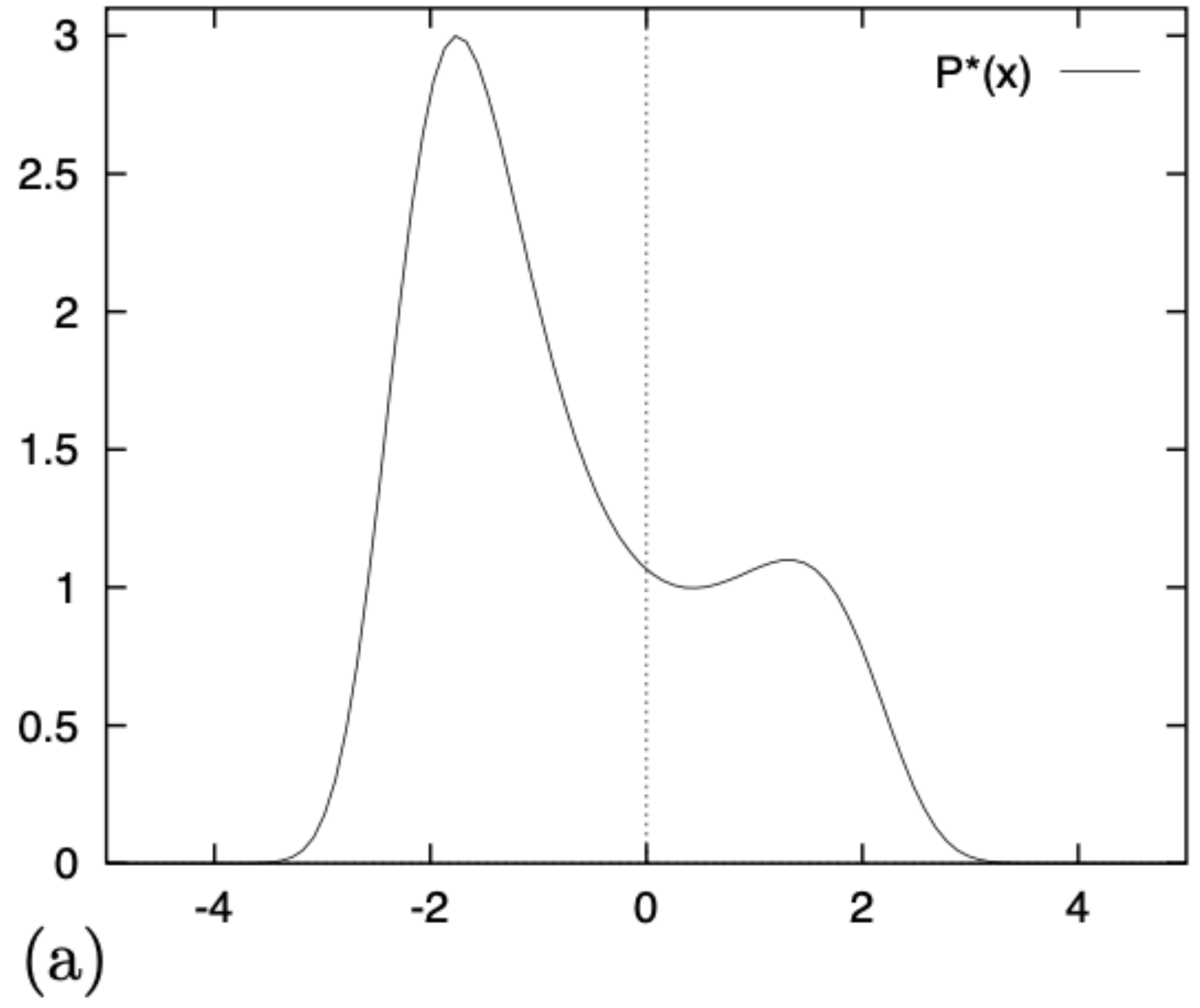
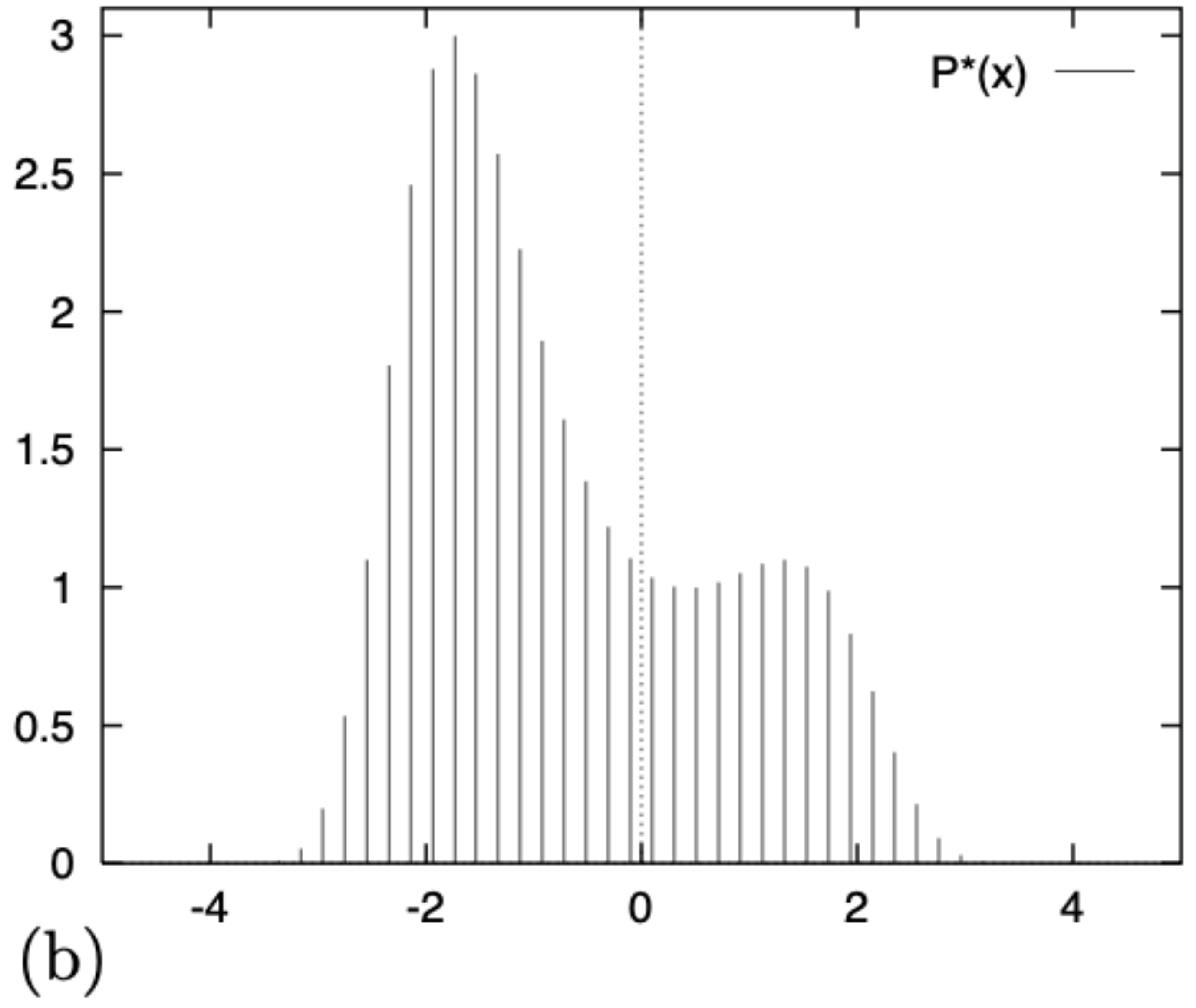
- We first need to know Z.





Monte Carlo methods

A simple 1D example

- Let's try with a brute-force approach: we can evaluate discretize $P^*(x)$ by evaluating it on equally spaced values $\{x^{(i)}\}$, and then compute:

$$Z = \sum_i P^*(x^{(i)}) \rightarrow P(x^{(i)}) = P^*(x^{(i)})/Z$$

- We can now sample from $P(x^{(i)})$. A basic sampling algorithm would just be to draw many times a number in $U(0,1)$ and compare to $P(x^{(i)})$ for each $x_i \in \{x^{(i)}\}$.

Monte Carlo methods

A simple 1D example: computational cost

- To compute Z we have to visit every point in the space. Depending on the x spacing (n), and the number of dimensions (d), this operation requires n^d computations.

- A typical cosmological problem involves at least 6 parameters, and the typical spacing is ~1000 points. This means we need to perform $1000^6 \approx 10^{18}$ operations. A theory code for cosmological purposes (CAMB, CLASS) take ~1s (best scenario); this means a computer would take $10^{18}s \approx 30Gyrs$.

Monte Carlo methods

Uniform sampling

- Acknowledged that we can't exhaustively visit every location x in the parameter space, let's try to solve the second problem: **estimating the expectation of a function** $\phi(x)$.

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- We could try to draw random samples of $\{x^{(i)}\}_{i \in N}$ uniformly and evaluate $P^*(x^{(i)})$ at those points.
- We can then normalize by $Z_N = \sum_{i=1}^{N} P^*(x^{(i)})$ and estimate $\Phi(x) = \int \phi(x) P(x) dx$ via:

$$\hat{\Phi} = \sum_{i=1}^{N} \phi(x^{(i)}) \frac{P^*(x^{(i)})}{Z_N}$$

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Monte Carlo methods

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- Each sample has a chance $2^H/2^d$ to fall in the typical set. We therefore need at least $N \approx 2^{d-H}$ samples.
- **This means that unless $H \sim d$, or $P(x)$ is uniform, corresponding to quite boring cases, uniform sampling is unlikely to be useful, or efficient.**

Monte Carlo methods

overview

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We need some workaround.

Monte Carlo methods

Importance Sampling

Let’s try to make the uniform sampling a little bit more general.

- Let’s assume a target distribution $P(x)$ we are able to evaluate at each x:

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- But $P(x)$ is too complicated to sample directly from it…

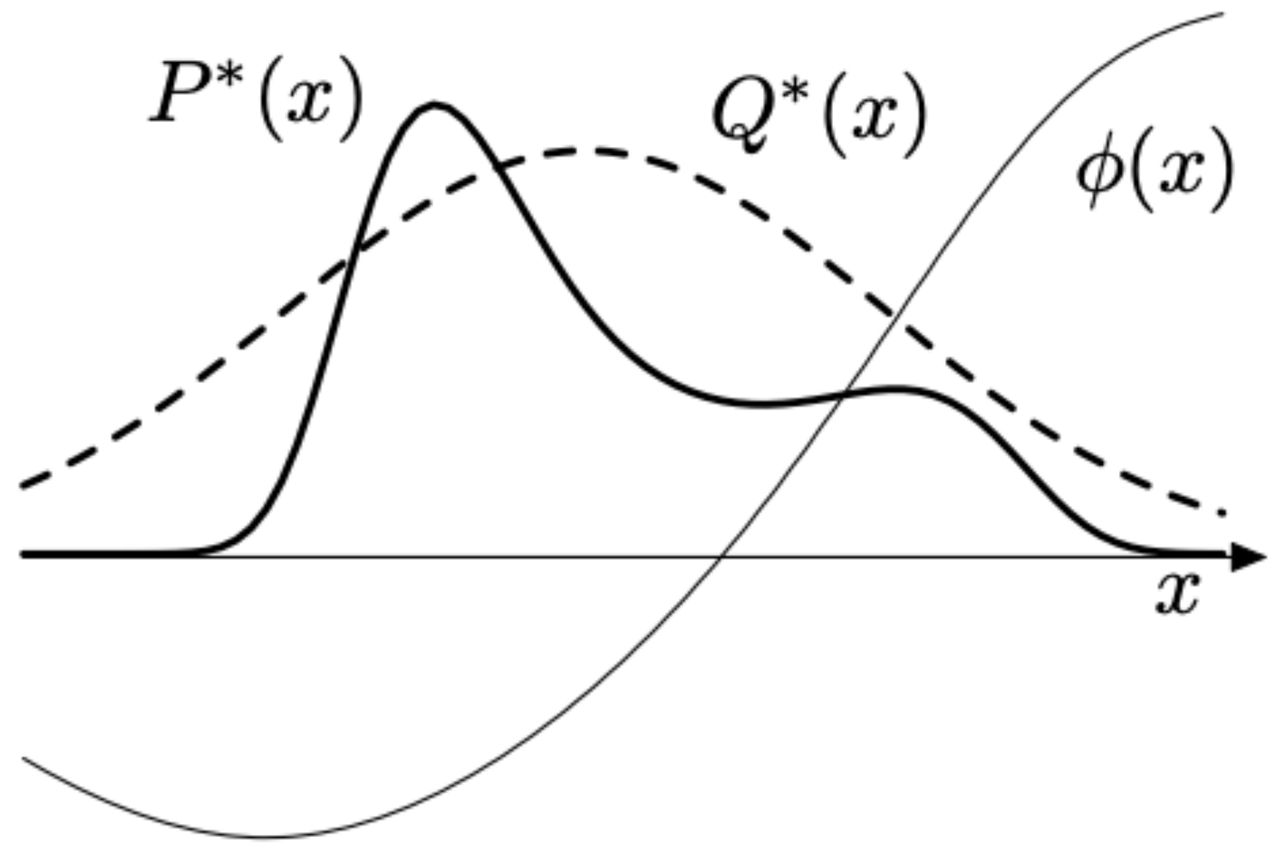
- But let's assume we have a simpler density $Q(x)$, from which we can generate samples and which we can evaluate up to a normalization constant:

$$Q(x) = Q^*(x)/Z$$

Monte Carlo methods

Importance Sampling

- We can generate N samples from $Q(x)$.



Monte Carlo methods

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- We can generate N samples from $Q(x)$.
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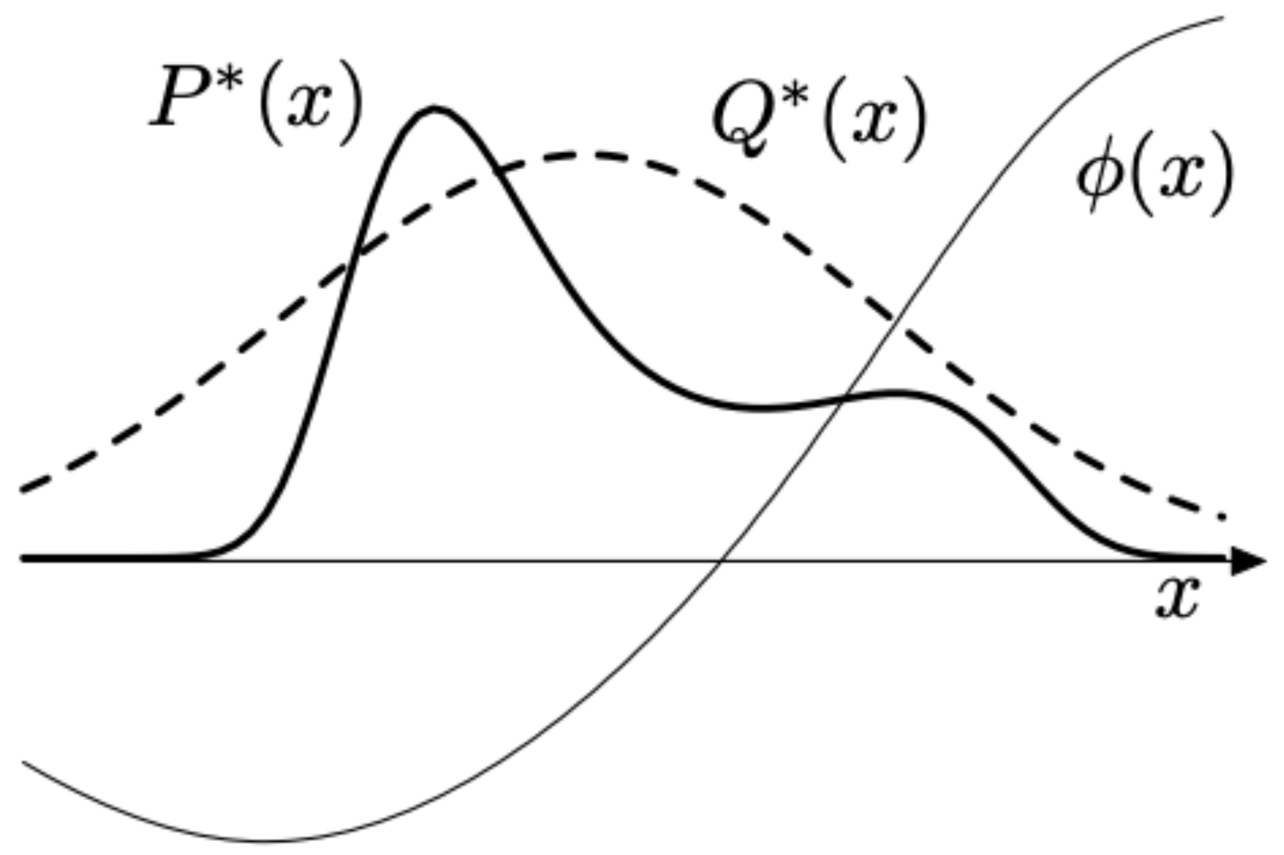
$$w^{(i)} = \frac{P^*(x^{(i)})}{Q^*(x^{(i)})}$$



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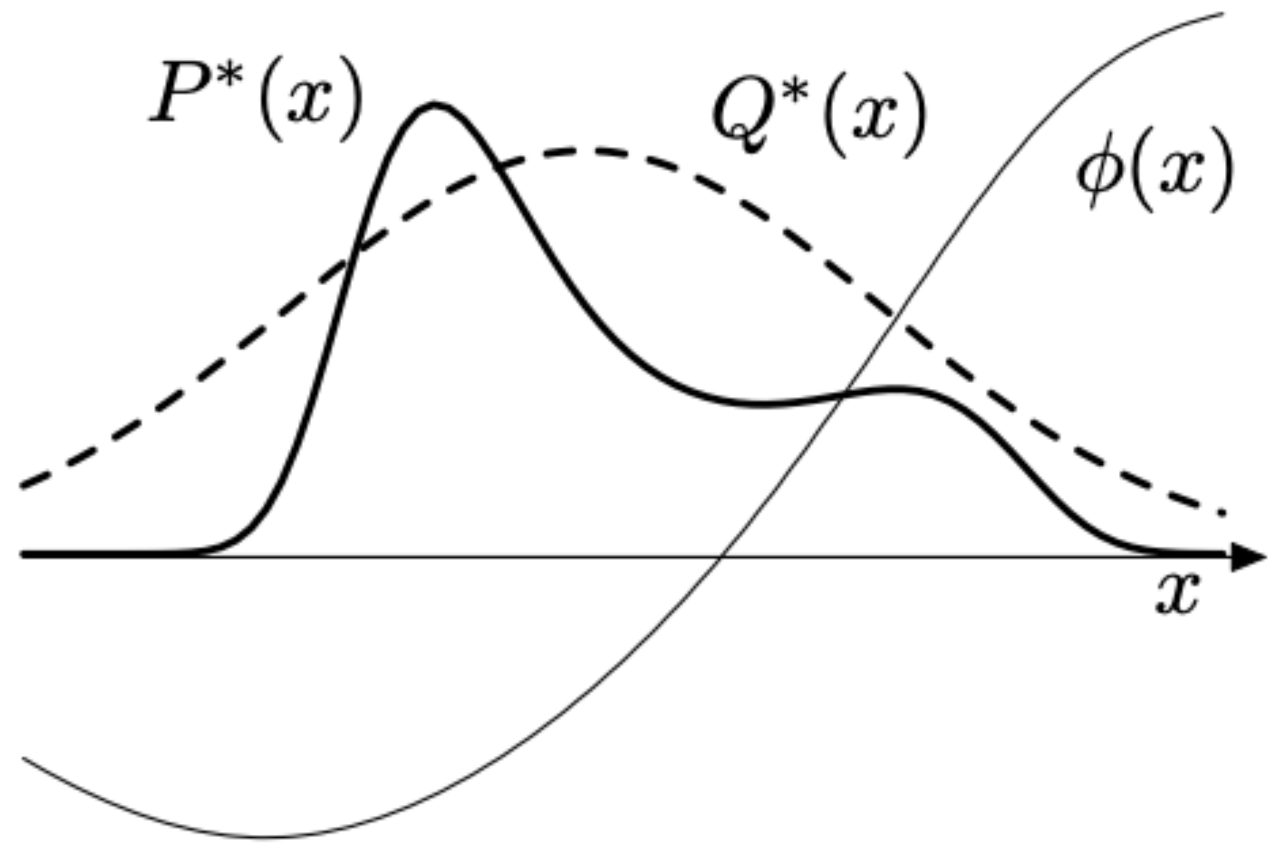
- Which we can use to adjust the importance of each point in our estimator such that:

$$\hat{\Phi} = \frac{\sum_i w^{(i)} \phi(x^{(i)})}{\sum_i w^{(i)}}$$



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Importance Sampling

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Monte Carlo methods

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Monte Carlo methods

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Drawbacks of importance sampling:

- It is hard to estimate how reliable $\hat{\Phi}$ is.
- The variance of the estimator is hard to estimate because it depends on an integral over x and $P^*(x)$.
- The variance of $\hat{\Phi}$ is not trivial because only relies on the empirical variances of $w^{(i)}$ and $w^{(i)}\phi(x^{(i)})$.

Monte Carlo methods

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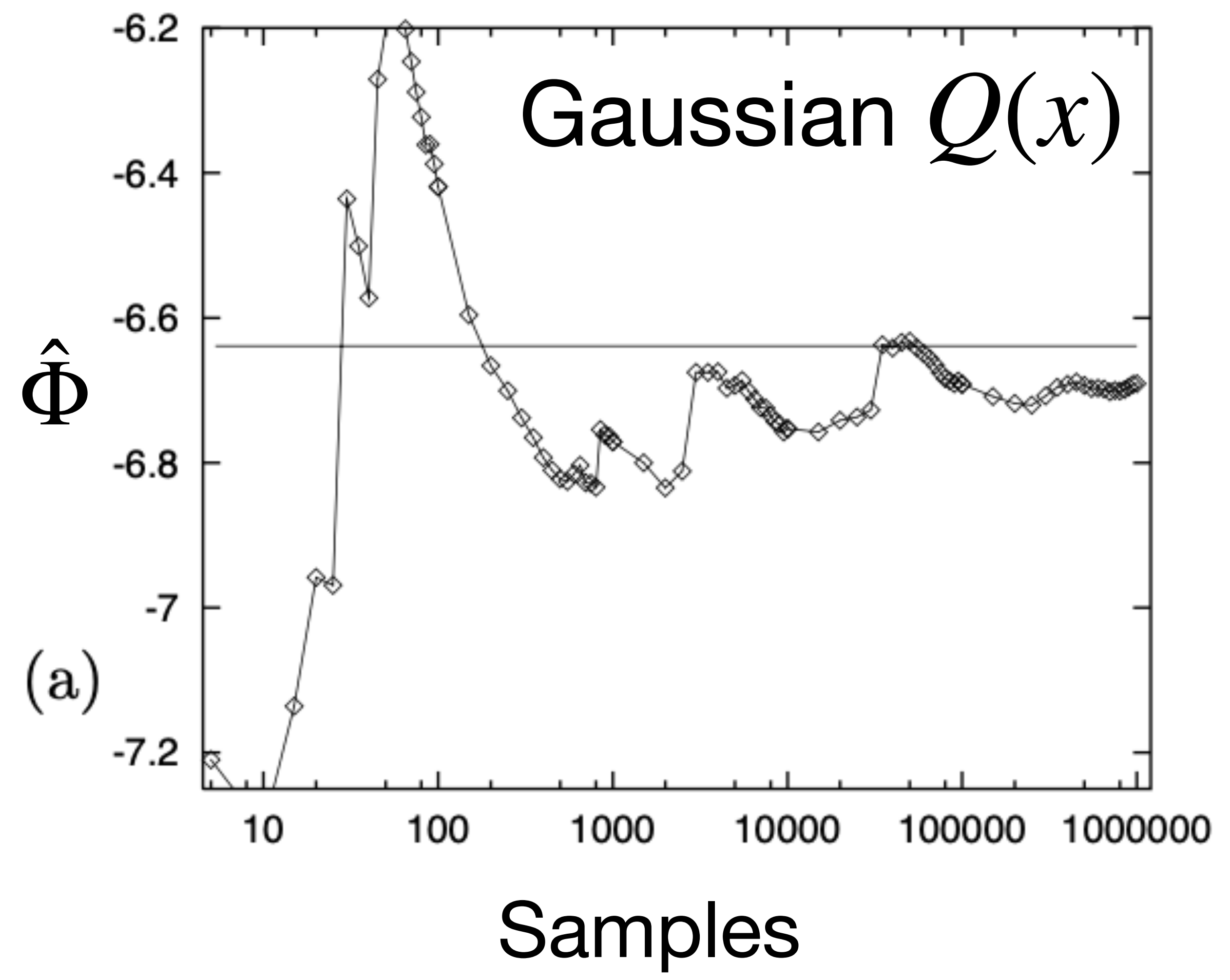

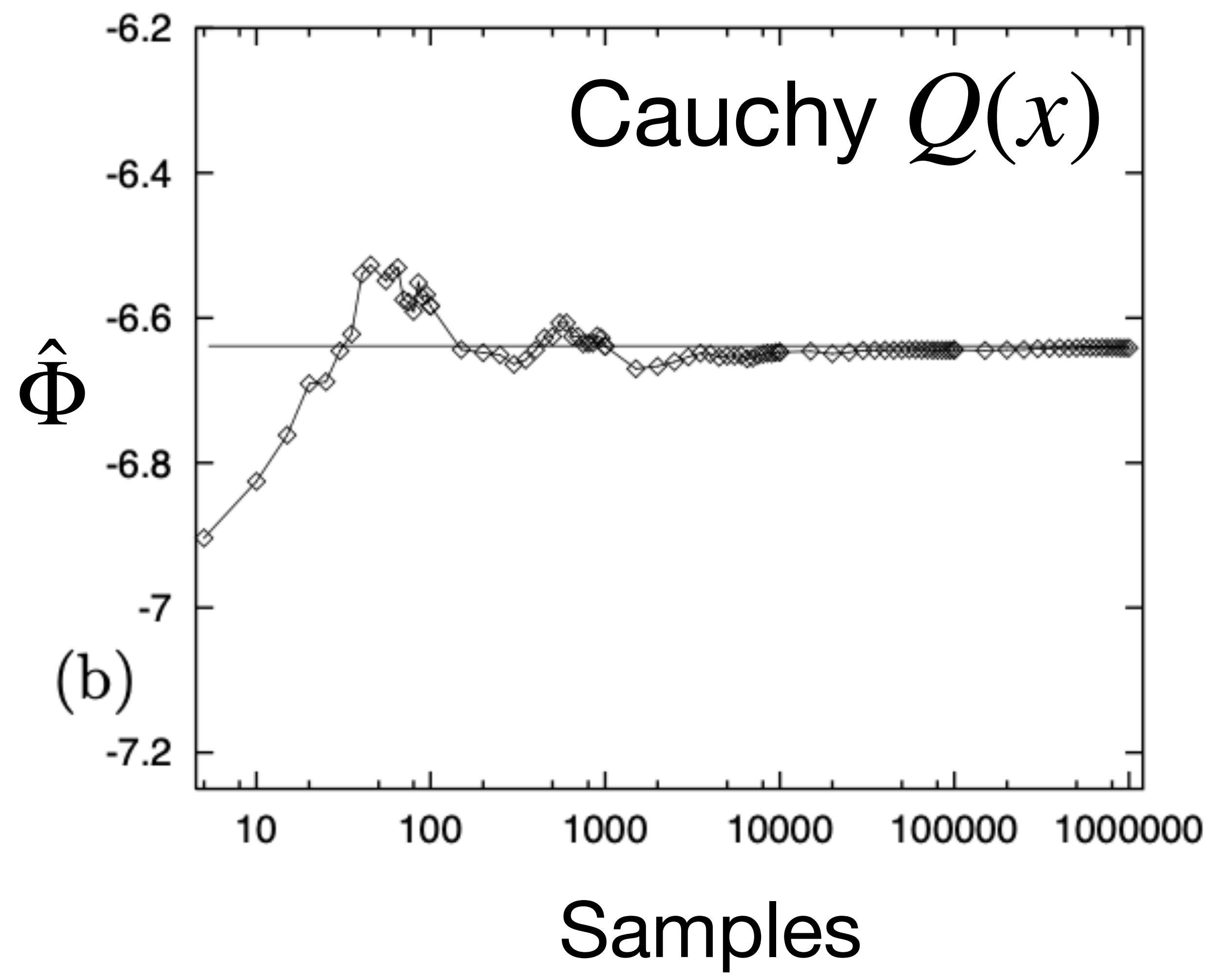

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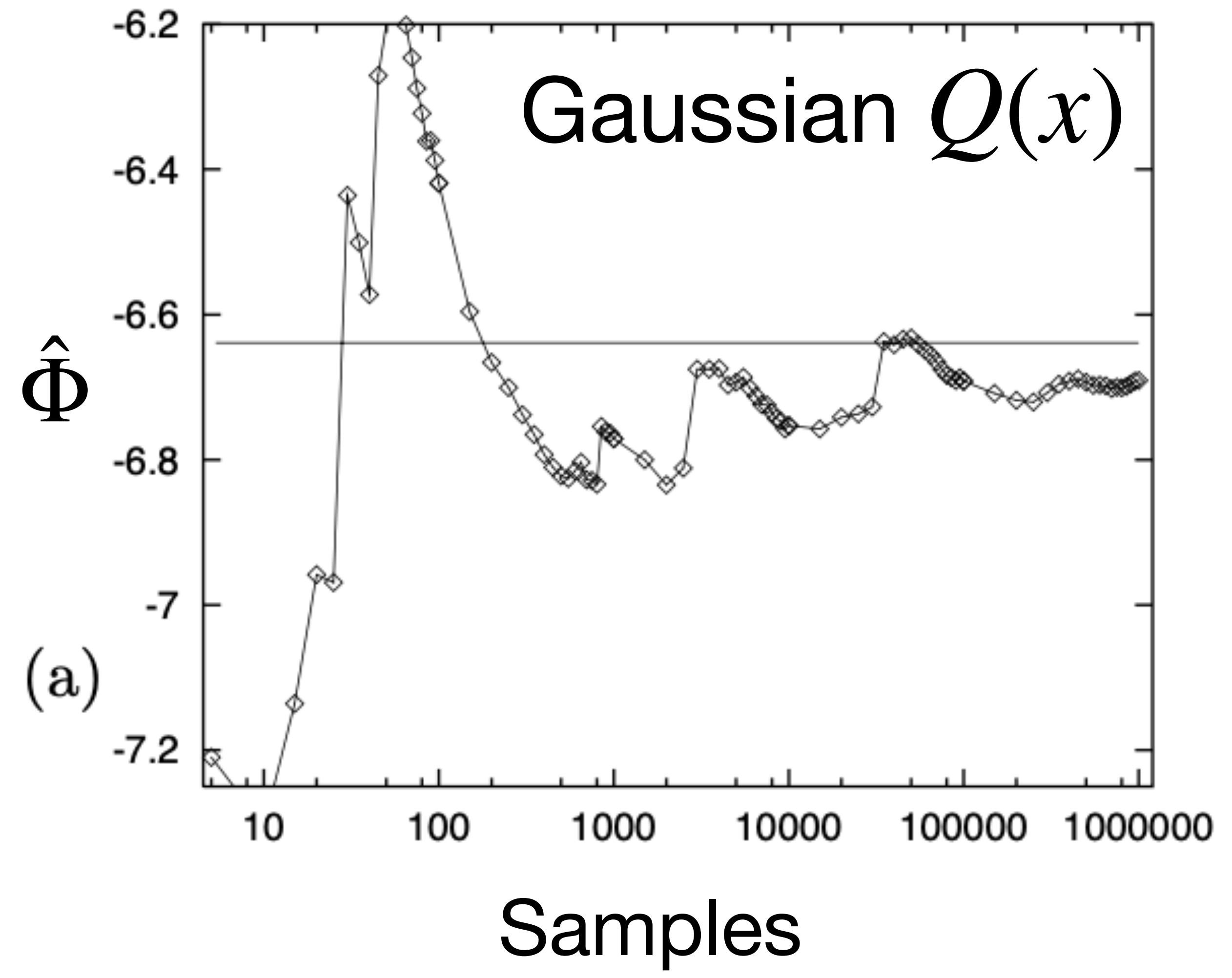

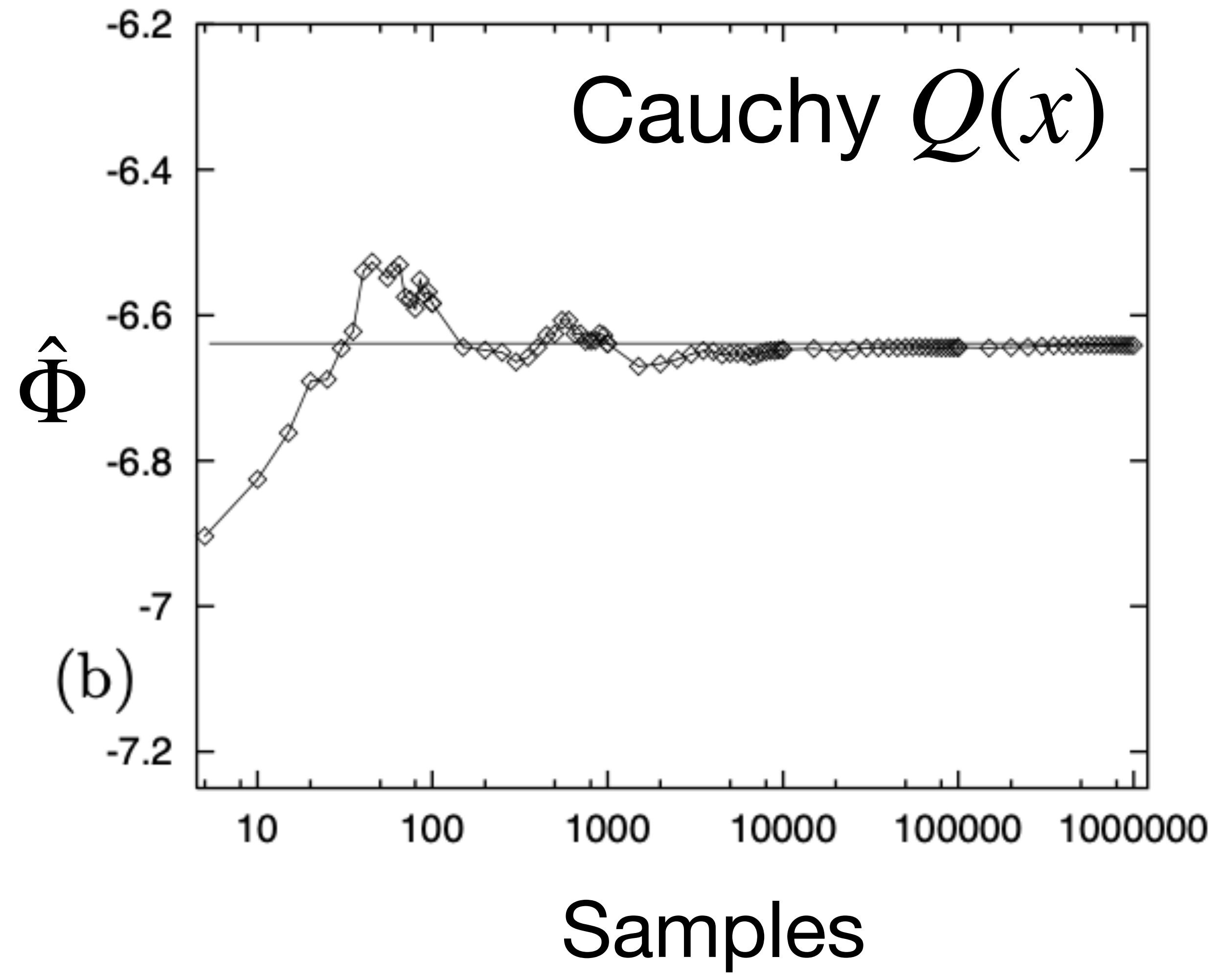

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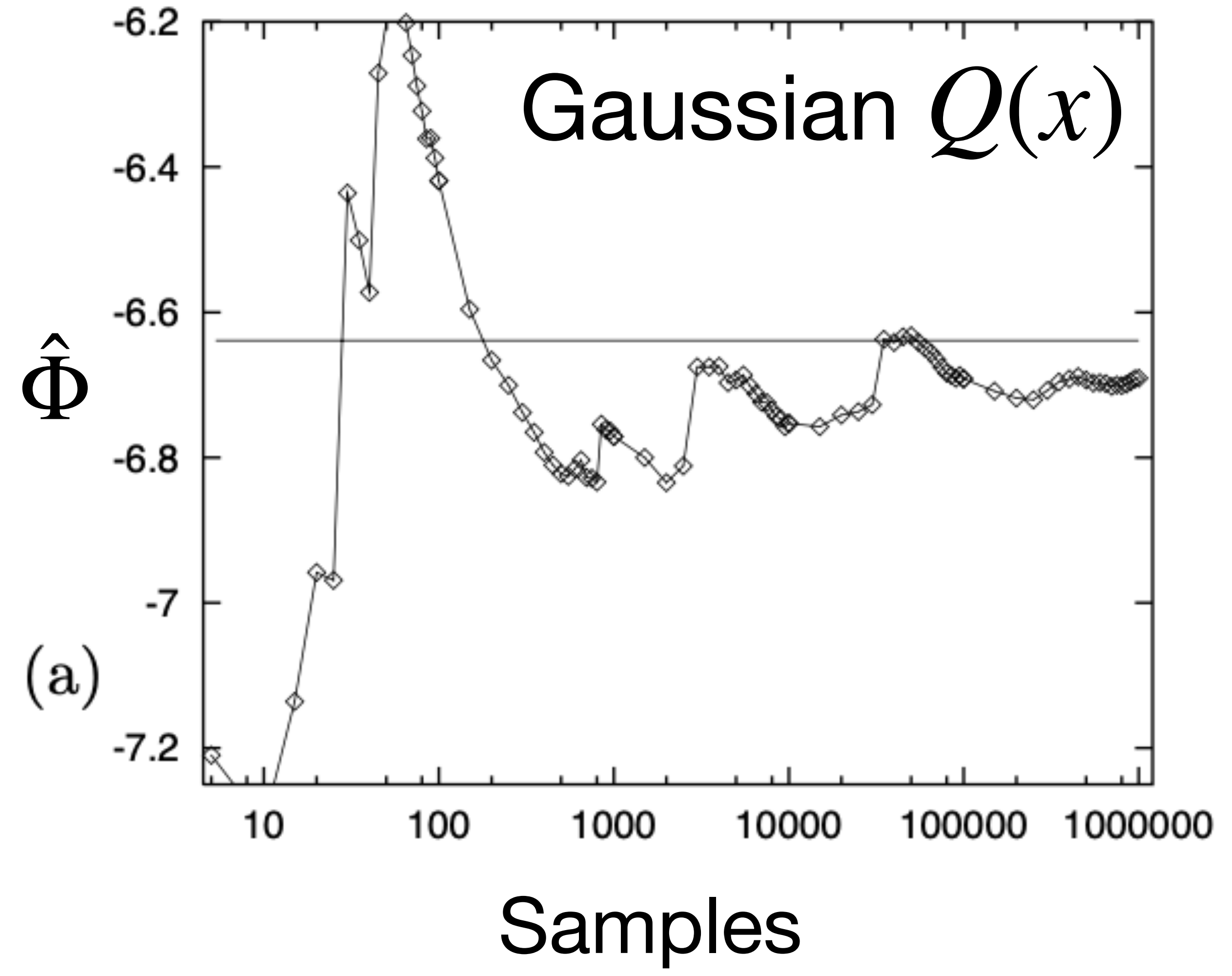
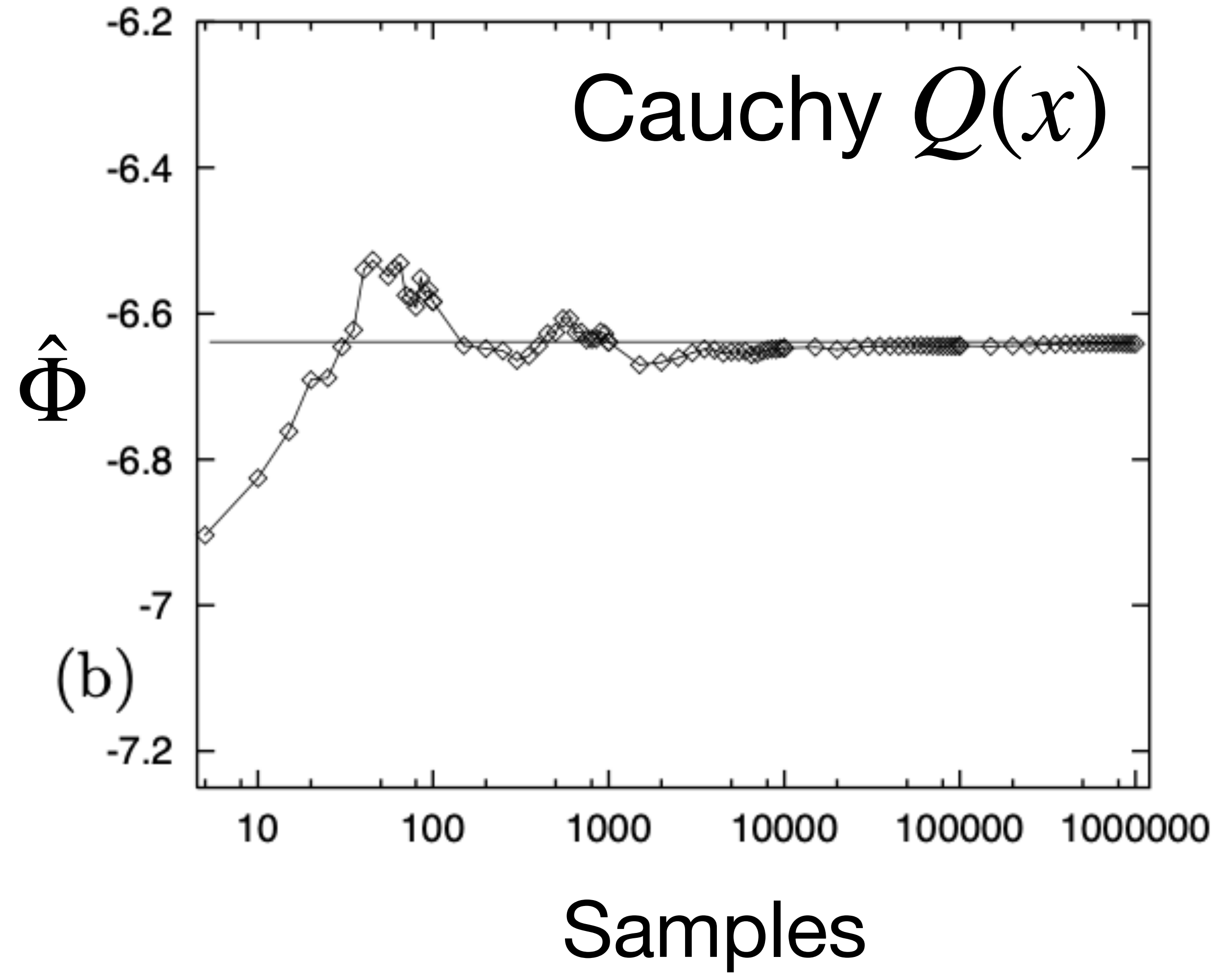
- The variance of $\hat{\Phi}$ is not trivial because only relies on the empirical variances of w_i and $w_i\phi(x_i)$.
    - If the $Q(x)$ is small where $|\phi(x)P^*(x)|$ is large, it may happen that, even for a large number of samples, none of them will fall in that region.





Monte Carlo methods

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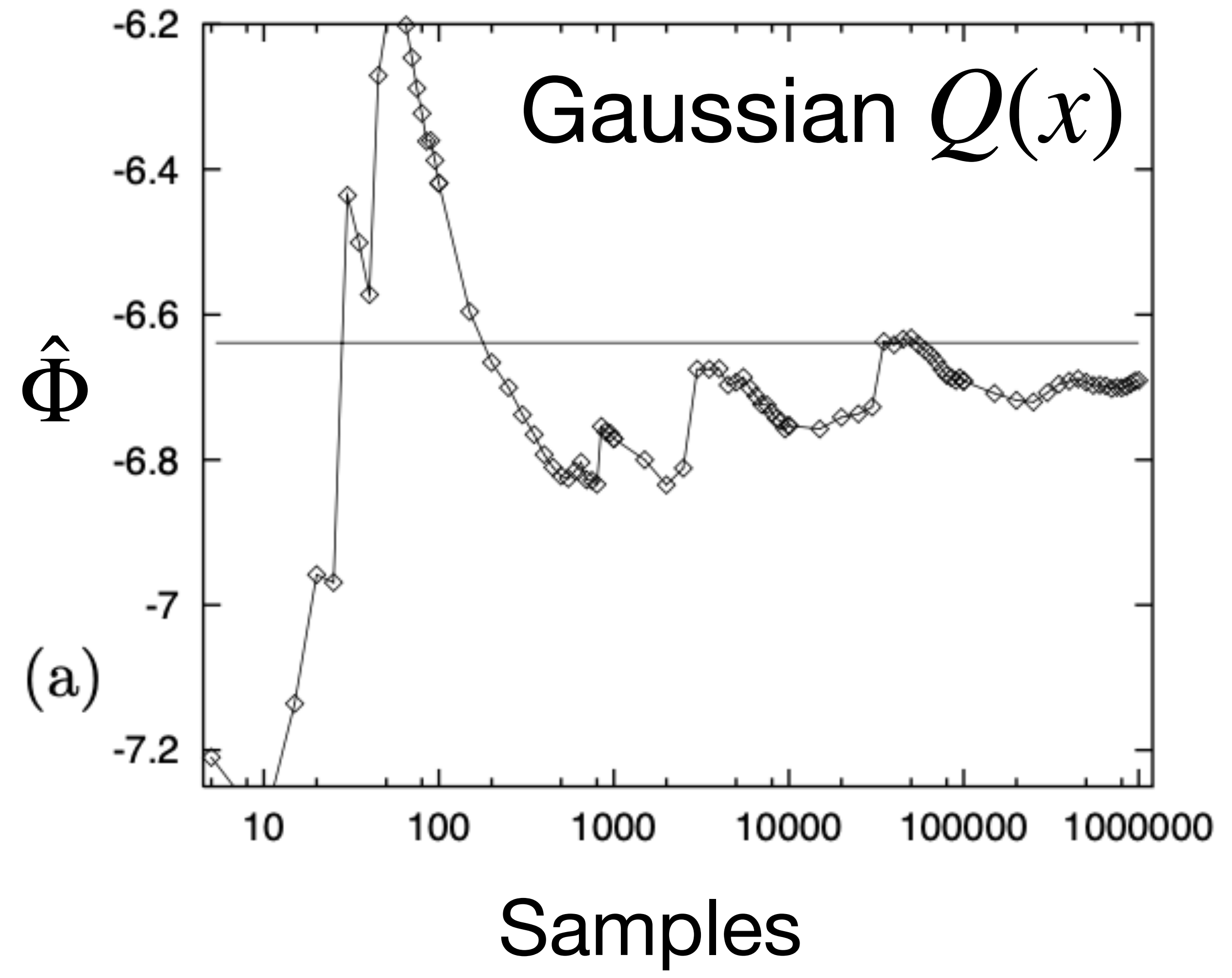
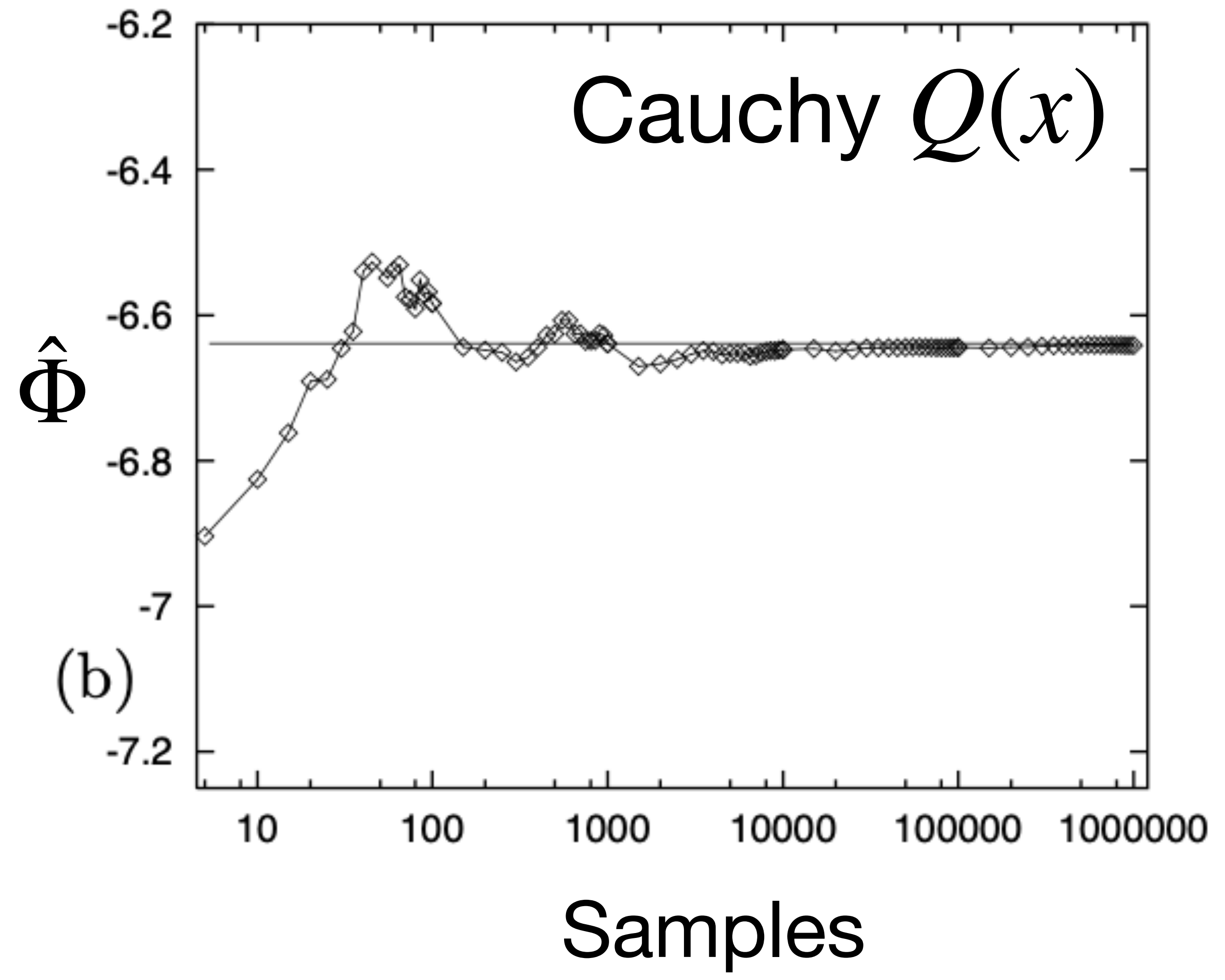
  - If the $Q(x)$ is small where $|\phi(x)P^*(x)|$ is large, it may happen that, even for a large number of samples, none of them will fall in that region.
  - In this case $\hat{\Phi}$ will be wrong, with no indication in the empirical variance variance that the true variance of $\hat{\Phi}$ is large.





Monte Carlo methods

Rejection sampling

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Monte Carlo methods

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- We also assume that we know the value of a constant c such that:

$$cQ^*(x) > P^*(x)$$

Monte Carlo methods

Rejection sampling

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Monte Carlo methods

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Monte Carlo methods

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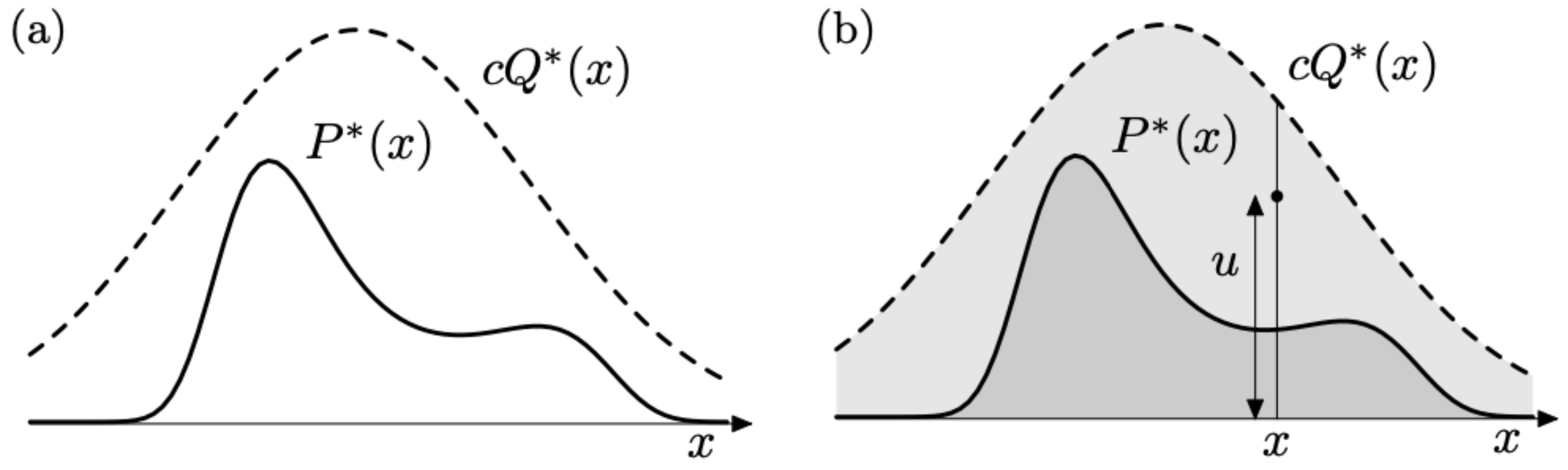
- We evaluate $cQ^*(x)$ and generate $u \sim U(0, cQ^*(x))$.
- We evaluate $P^*(x)$ and accept or reject x by comparing the value of u with $P^*(x)$. If $u > P^*(x)$ then x is rejected, otherwise is accepted and added to our collection of samples $\{x^{(i)}\}_N$.



Monte Carlo methods

Rejection sampling

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Rejection sampling

- This method works best if Q is a good approximation to P.

- If Q and P are very different, we need a very large value of c to ensure $cQ > P$ everywhere, and therefore the rejection frequency will be large —> need a lot of samples.

Markov chains

Definitions

- A sequence $X_1, X_2, \ldots, X_n$ of random elements of some set is a **Markov chain** if the conditional distribution of X_{n+1} given $X_1, \ldots, X_n$ depends on X_n only.
- A Markov chain has **stationary transition probabilities** if $P(X_{n+1} \,|\, X_n)$ does not depend on n.

Markov chains

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Markov chains

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Moreover:

Markov chains

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- The marginal distribution of X_1, called the **initial distribution**.
- $P(X_{n+1} \,|\, X_n)$, called the **transition probability distribution**.

Moreover:

- A transition probability distribution is **reversible** with respect to an initial distribution if, for the Markov chain $X_1, X_2, \ldots$, the distribution of pairs m (X_i, X_{i+1}) is exchangeable.

Markov chains

Reversibility

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- The Markov chain Central Limit theorem is much sharper and conditions much simpler when reversibility applies.

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Reversibility plays two roles in Markov chain theory:

- The Markov chain Central Limit theorem is much sharper and conditions much simpler when reversibility applies.

- It allows for constructing efficient probability mechanisms for MCMC (we'll see shortly…).

MCMC algoritms

Metropolis-Hastings

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MCMC algoritms

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- This is an MCMC process, and $Q(x'; x^{(i)})$ does not need to be close to the true $P(x)$ to be useful!

Let's assume we can evaluate $P*(x)$ at any given x. How do we draw a new sample x' from the proposal density $Q(x'; x^{(i)})$?

MCMC algoritms

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Note the difference from rejection sampling: here a rejection cause the current state to be written again into the samples list.

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Gibbs sampling can be viewed as a MH method in which a sequence of proposal distributions Q are defined in terms of the conditional distributions of the joint distribution $P(\mathbf{x})$.

It is assumed that $P(\mathbf{x})$ is too complex to draw samples from, but its conditional distributions $P(x_i \,|\, x_{j\neq i})$ are tractable to work with.

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MCMC algoritms

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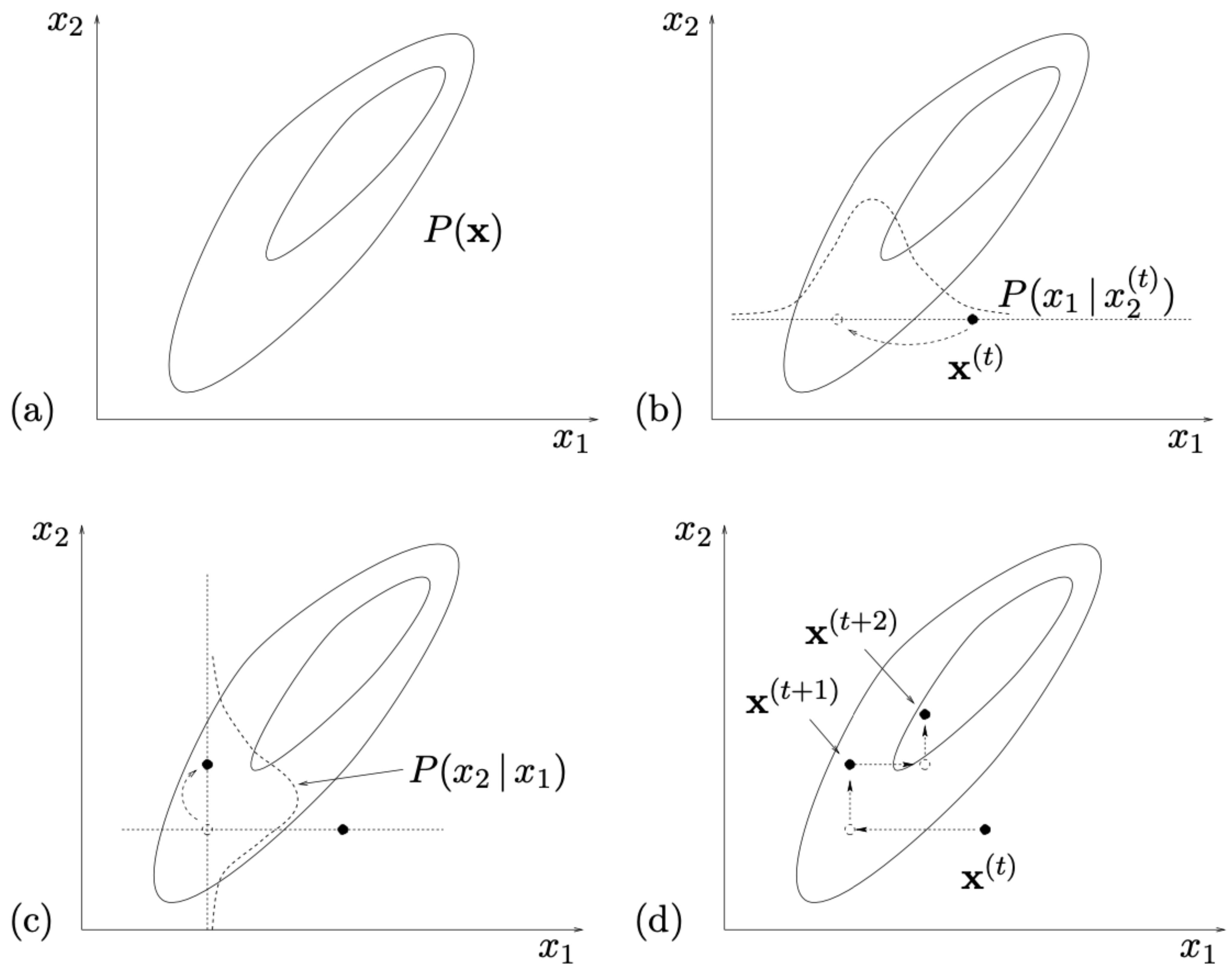
A simple 2D example:



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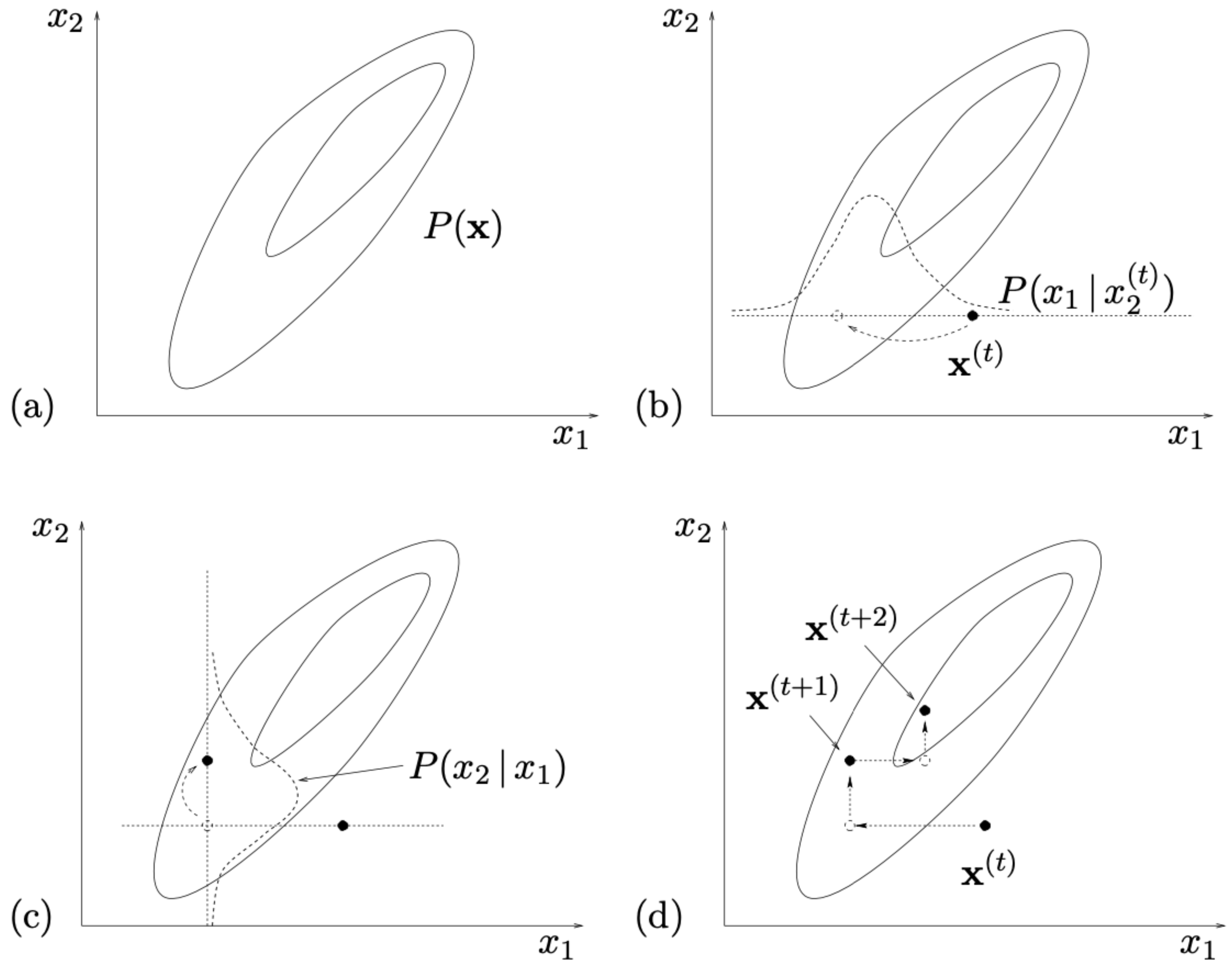

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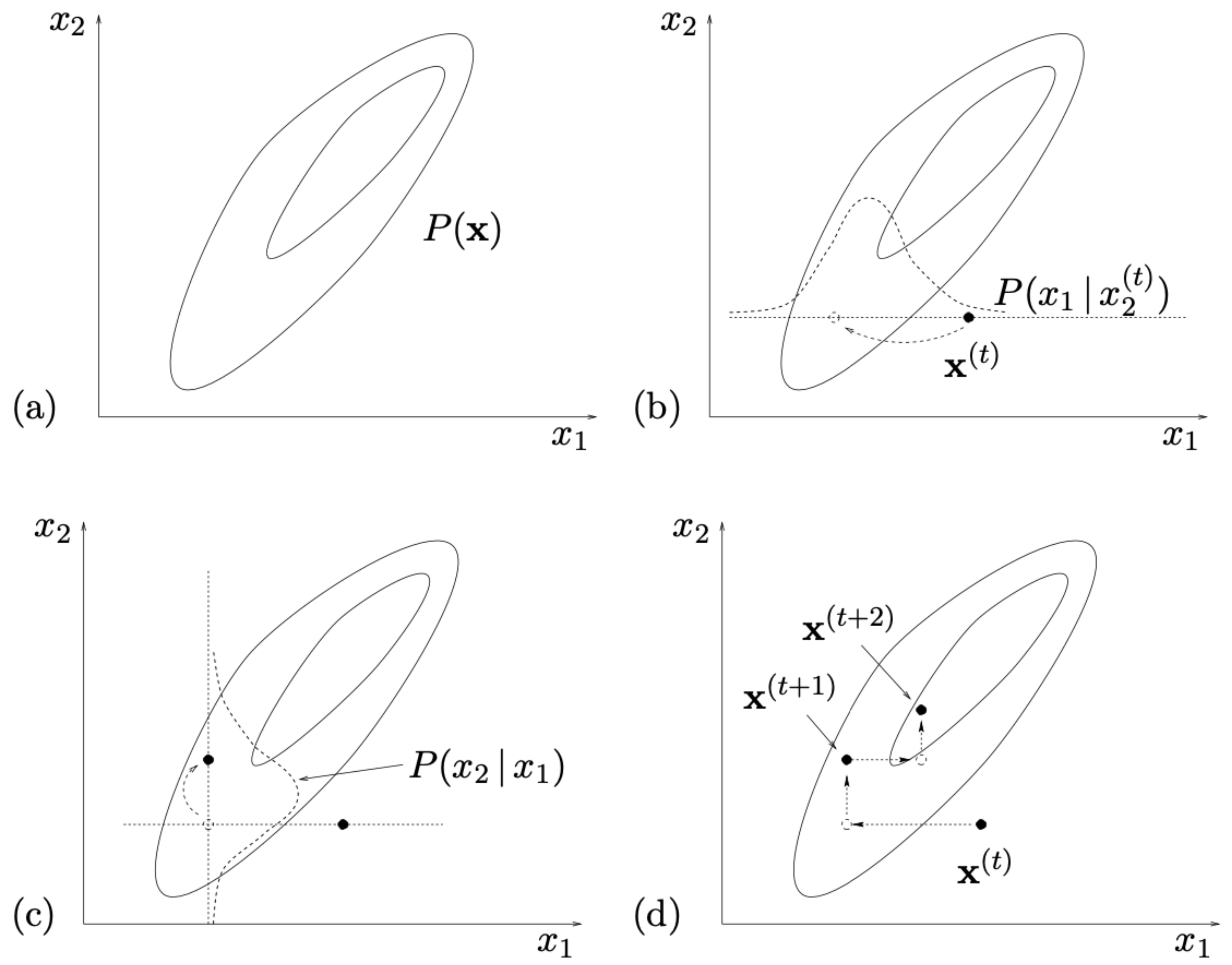

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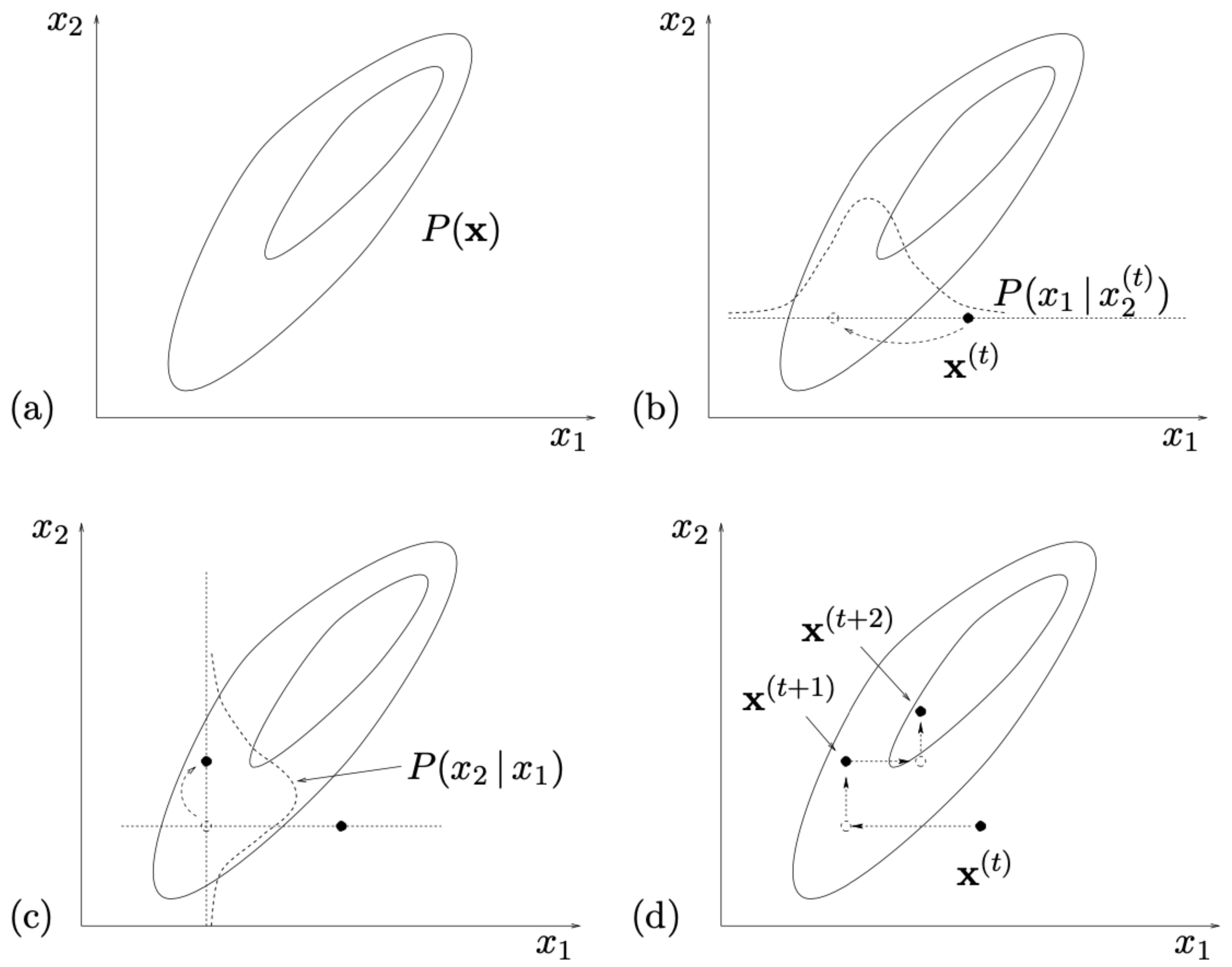

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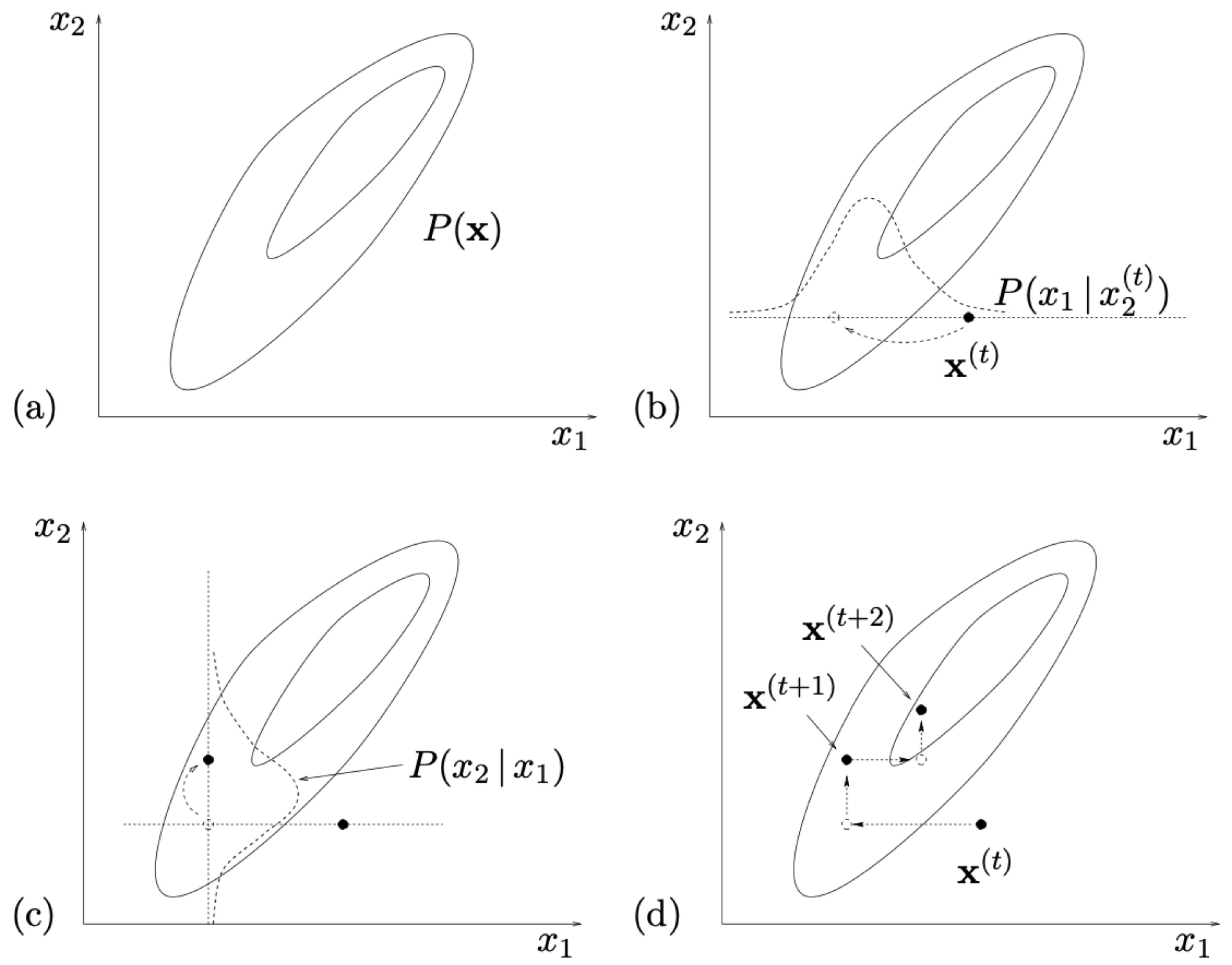

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In general, for a system of K variables, a single iteration involves sampling one parameter at a time:

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x_2^{(t+1)} &\sim P(x_2 \,|\, x_1^{(t+1)}, x_3^{(t)}, \dots, x_K^{(t)}) \\
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Gibbs samples are always accepted!

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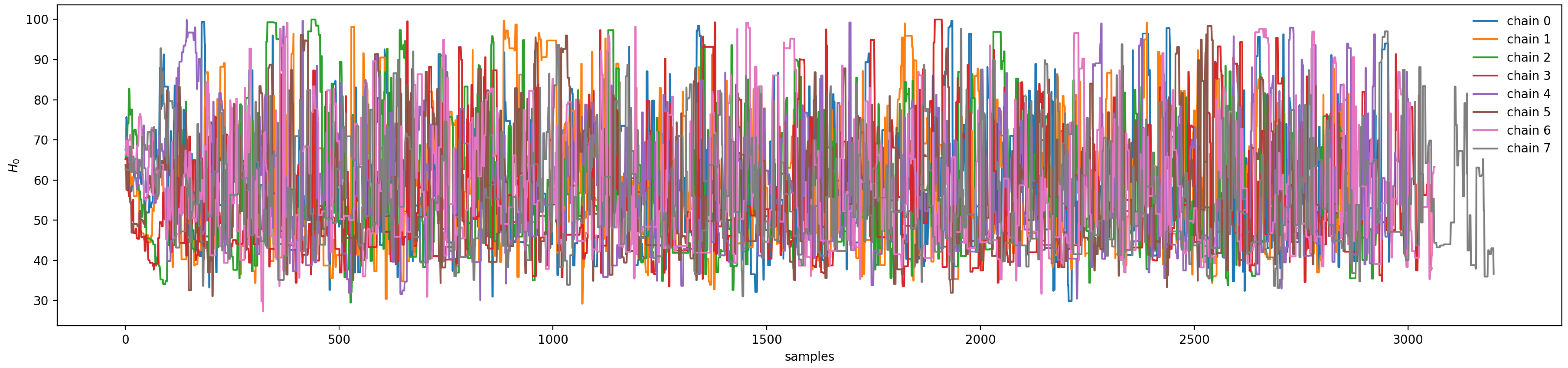
MCMC algoritms

Let’s play

- https://chi-feng.github.io/mcmc-demo/app.html

When to stop sampling?

First approach: by eye.



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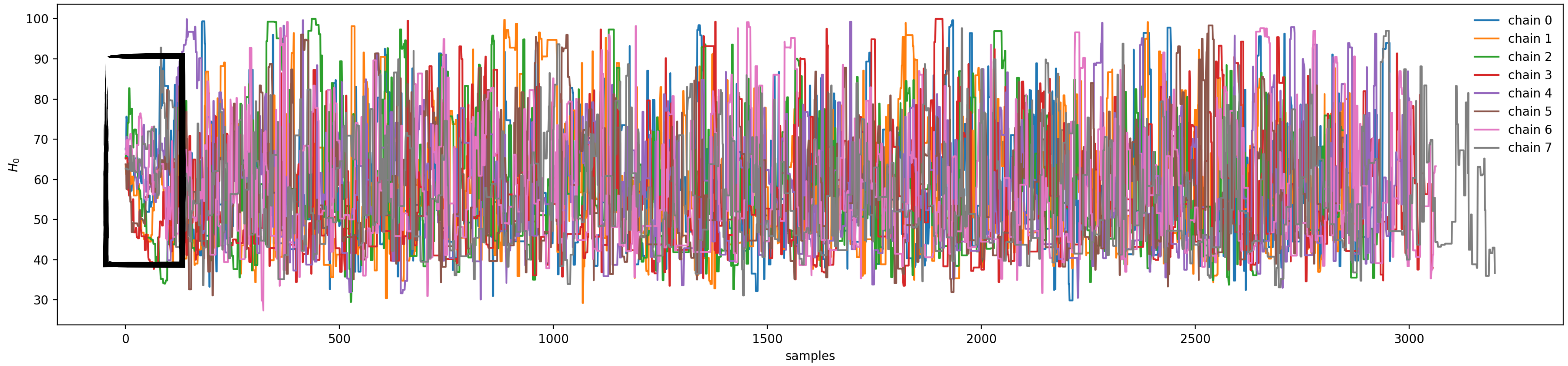

First Burn-in phase: chains leading to a stationary state from initial random points

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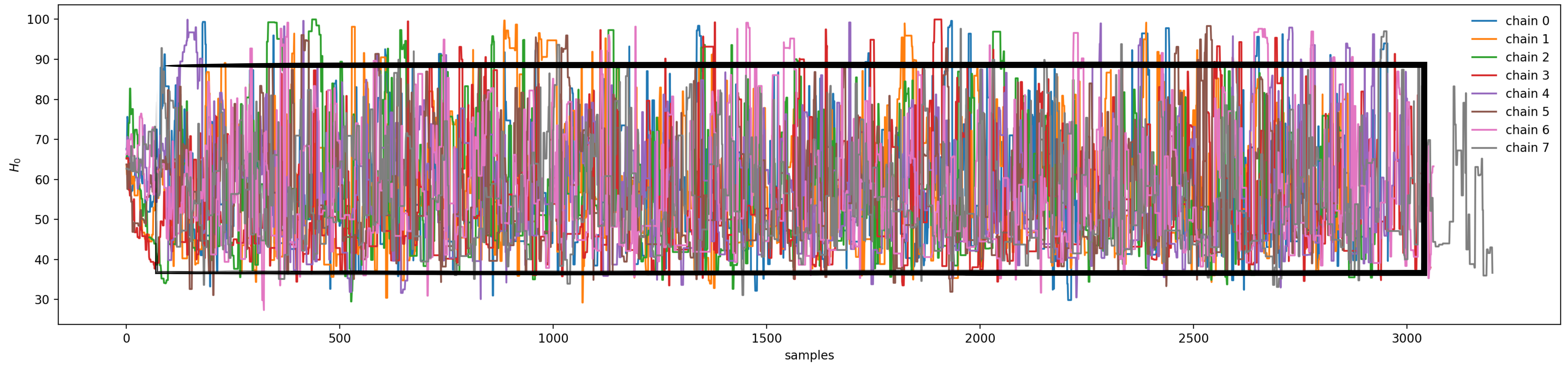
For a sufficiently long run all chains explore efficiently the parameter space.



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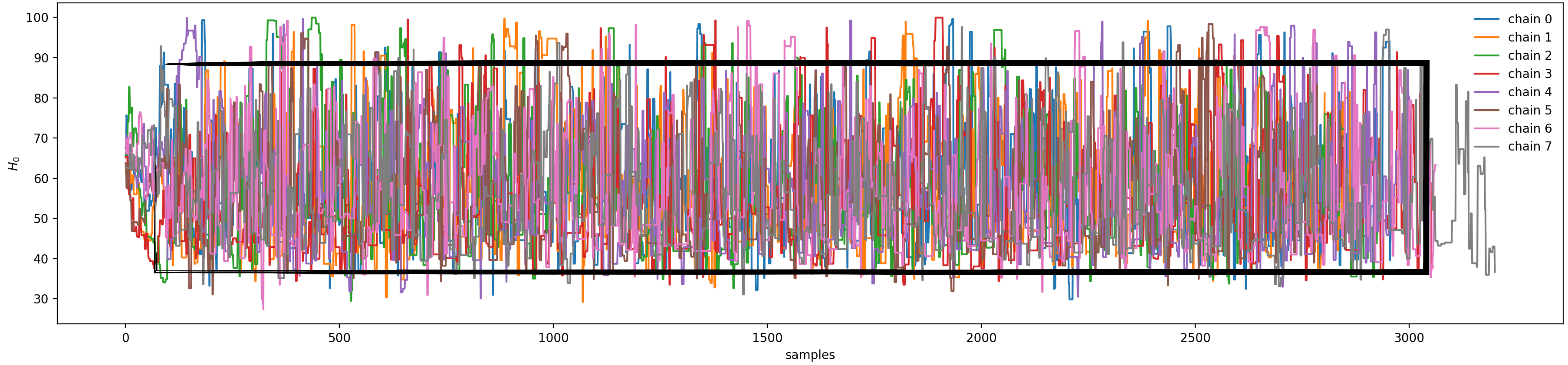

Small correlation length —> good exploration; ergodicity.

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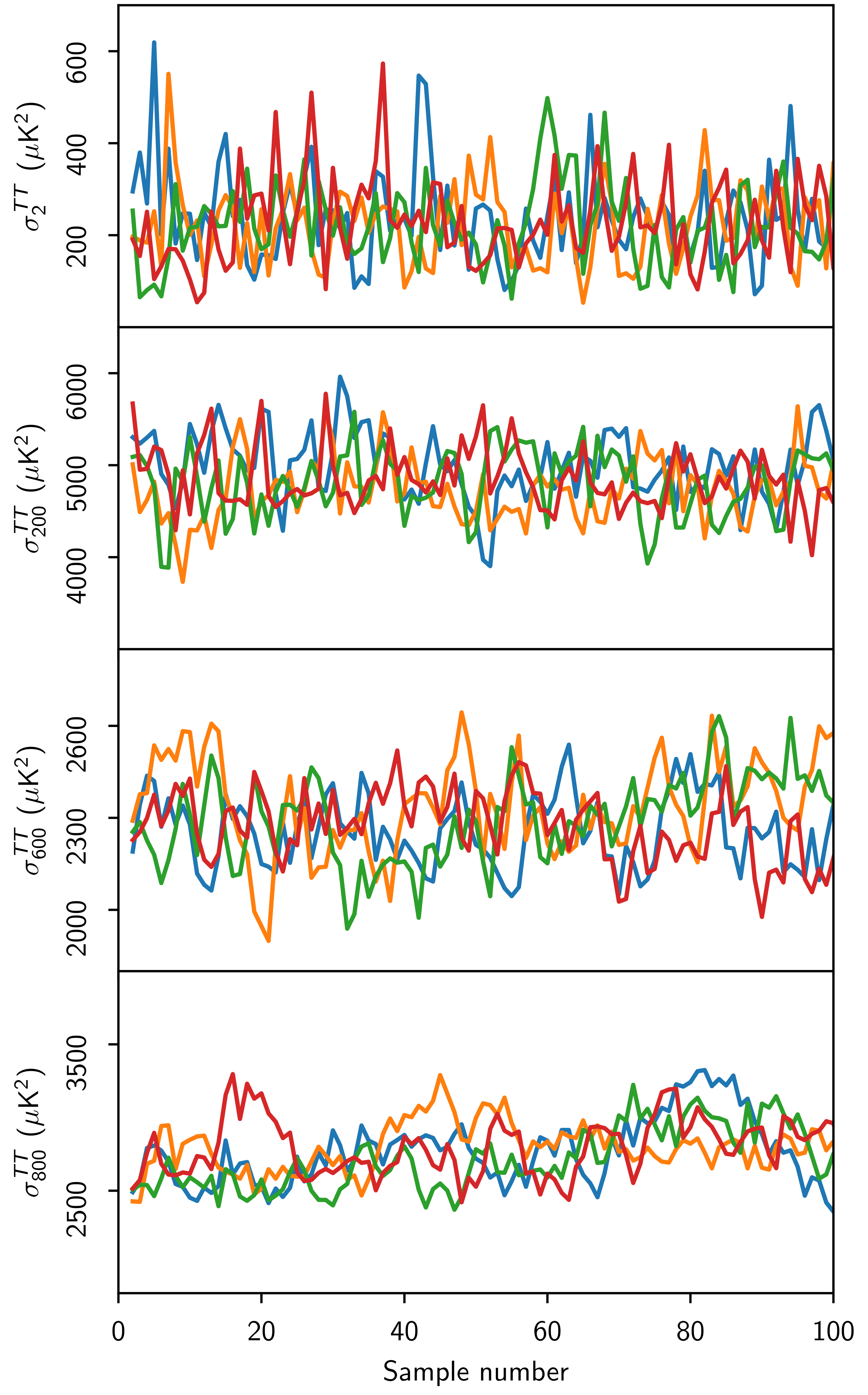
Correlation length can be very helpful when it comes to assess quickly the convergency status of chains **individually**.

BeyondPlanck I - The BeyondPlanck collaboration. 2023



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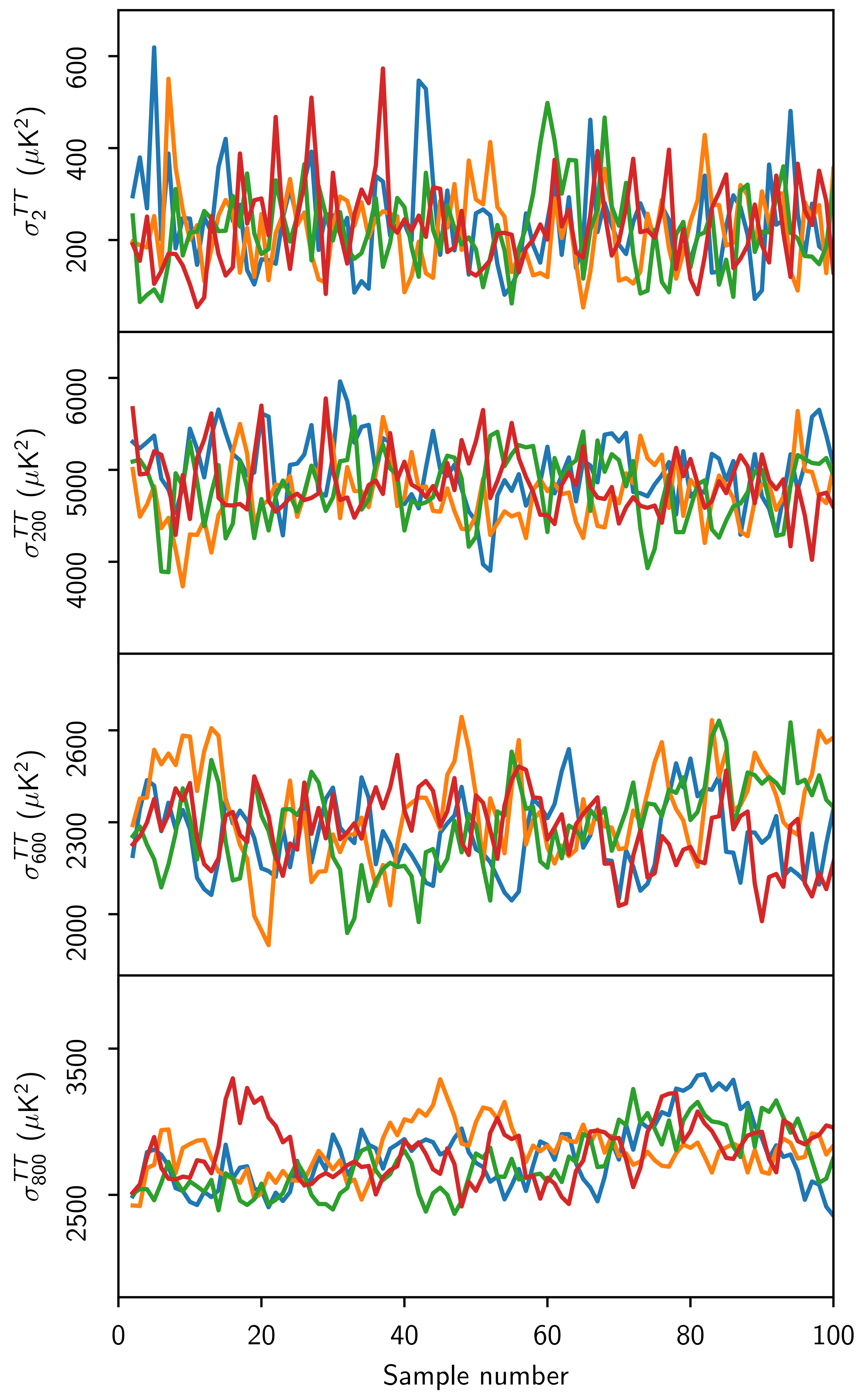

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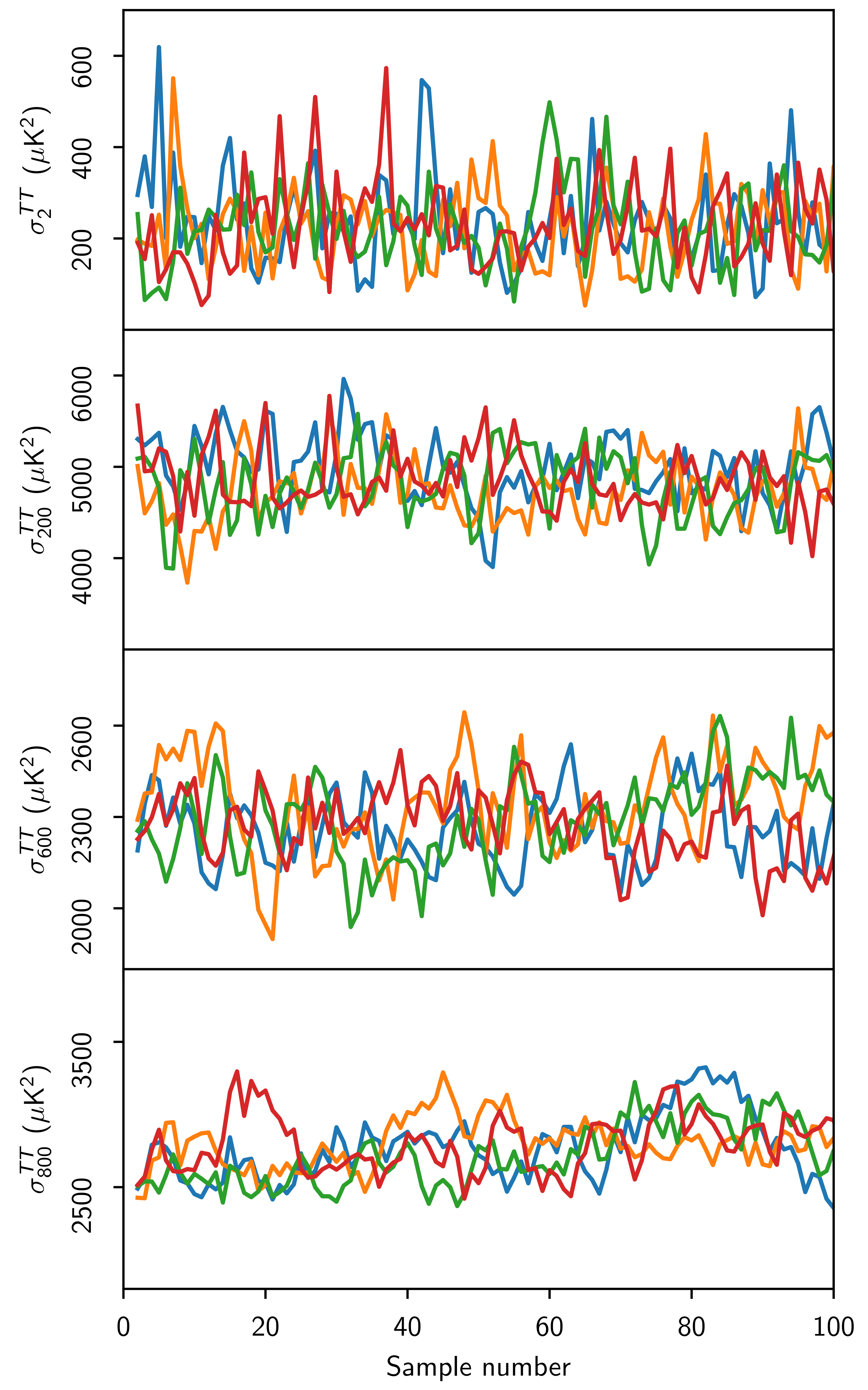

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However, parameters can be highly degenerate, and correlation length can just stay long —> **need much more samples** to properly explore the parameter space. This also **depends on the sampling algorithm**.

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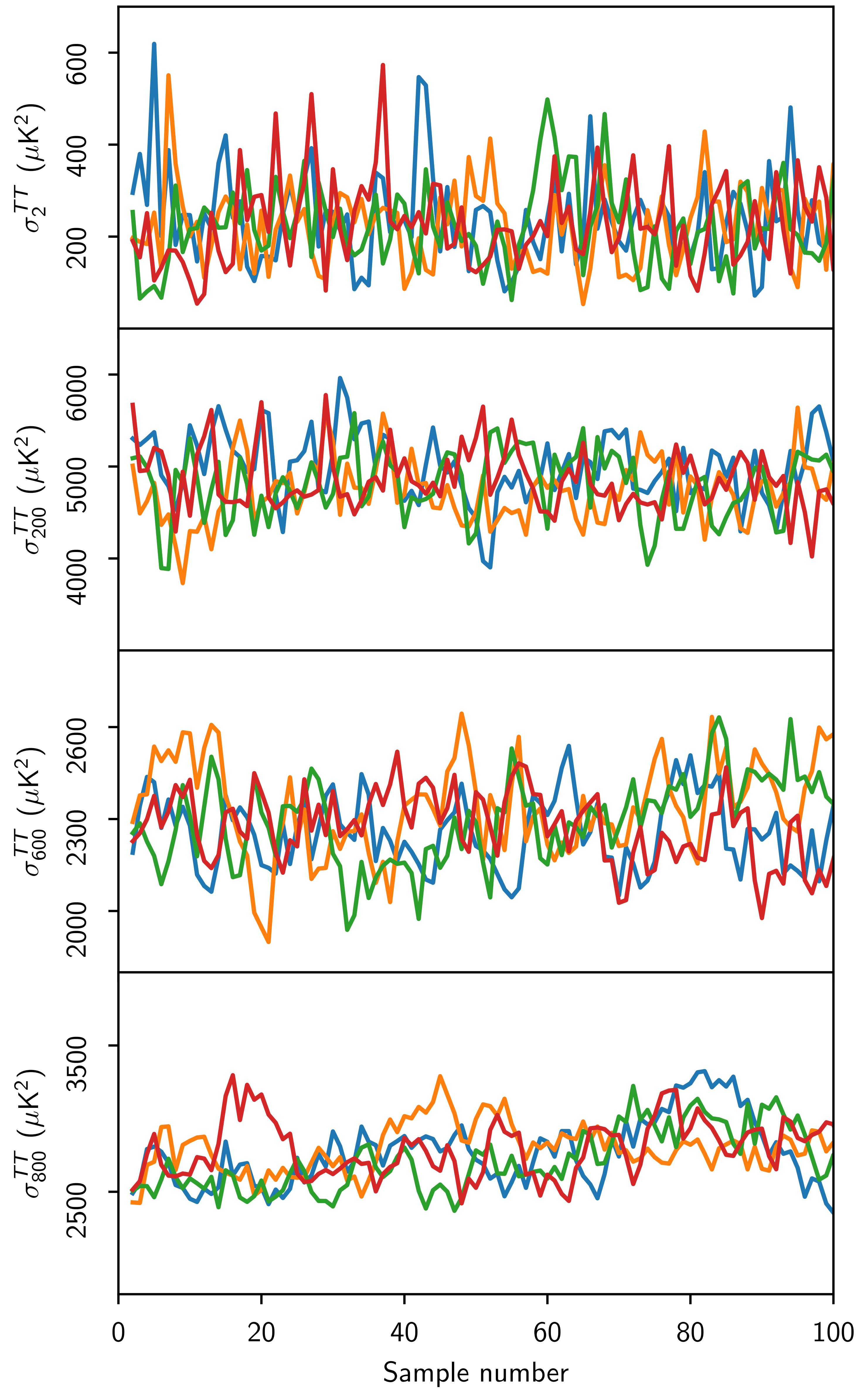

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$$\bar{x}_\cdot = \frac{1}{J}\sum_{j=1}^{J} \bar{x}_j \qquad \text{(grand mean)}$$

$$B = \frac{L}{J-1}\sum_{j=1}^{J} (\bar{x}_j - \bar{x}_\cdot)^2 \qquad \text{(between chain variance)}$$

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The GR diagnostic suggests that a good convergency is achieved for $R < 1.1$ or equivalently $R - 1 < 0.1$