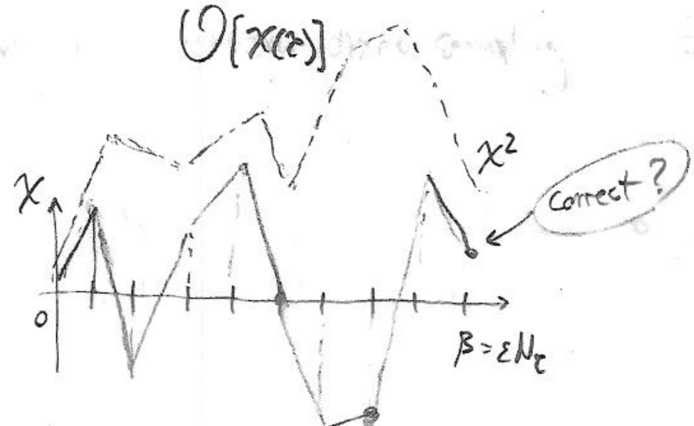
Recap from Monday

(I) Numerical (in particular stochastic) methods are necessary to determine the properties of interacting many-body quantum systems, because pert. theory and saddle point approximations can fail (and they do in many interesting cases).

(II) Stochastic methods use the path integral formulation of QM. This means that expectation values are computed like so:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_{x(0)=x(\beta)} \mathcal{D}[x(\tau)]\, e^{-S_E[x(\tau)]}\, \mathcal{O}[x(\tau)]$$



- Example: $\mathcal{O} = \frac{1}{\beta}\int_0^\beta x^2(\tau)\, d\tau$

(For each trajectory we compute $\frac{1}{\beta}\int_0^\beta x^2(\tau)\, d\tau$ and add it with weight $\frac{1}{Z}\exp\{-S_E[x(\tau)]\}$)

Get notation right!

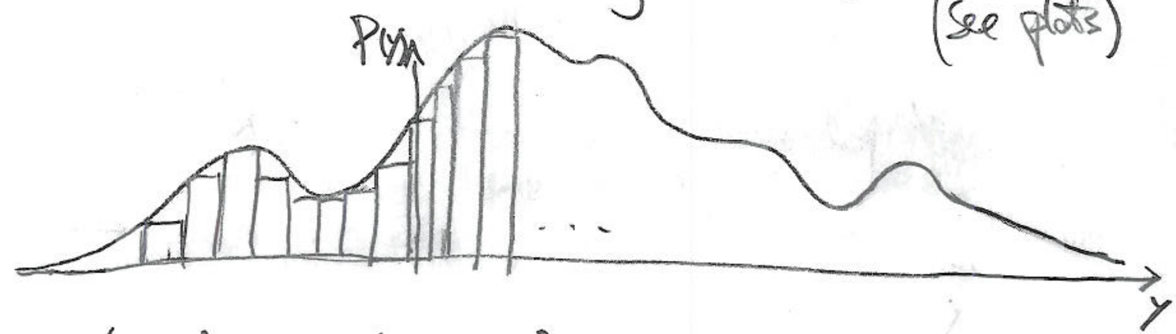
III Stochastic methods are based on the <u>central limit theorem</u>

Example: Consider y distributed according to $P(y)$

$P(y) > 0$

$\int P(y)dy = 1$

(see plots)



Drawing samples of y according to $P(y)$ and putting them in bins according to their value will eventually reproduce $P(y)$ as a histogram.

Now consider $\langle O \rangle = \int dy\, O(y) P(y)$ = "True mean"

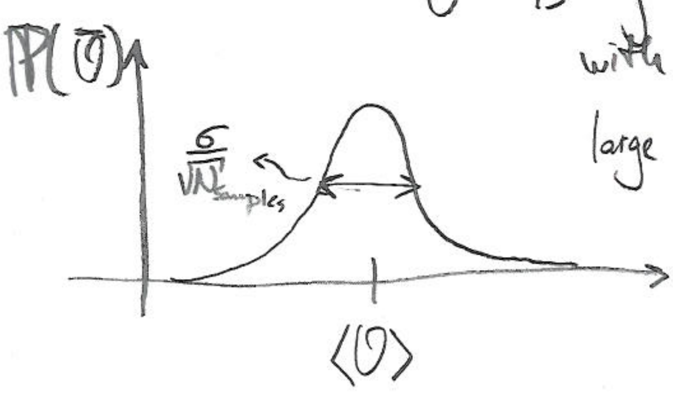
$\sigma^2 = \langle O^2 \rangle - \langle O \rangle^2$ = "True standard deviation" (squared)

Question: Can I approximate $\langle O \rangle \simeq \frac{1}{N_{samples}} \sum_{n=1}^{N_{samples}} O(y_n) \equiv \bar{O}$

taking y distributed according to $P(y)$?

(see plots)

CLT: Yes! $\bar{O}$ is "gaussianly distributed" around $\langle O \rangle$ (True mean) with std deviation $\frac{\sigma}{\sqrt{N_{samples}}}$, in the limit of large $N_{samples}$.



$\Rightarrow \langle O \rangle \simeq \bar{O} \pm \frac{\sigma}{\sqrt{N_{samples}}}$

We don't know the true $\langle O \rangle$, so this theorem tells us how to estimate it.

We also don't know the true σ, but we can estimate it as

$$\sigma \simeq \overline{O^2} - \overline{O}^2$$

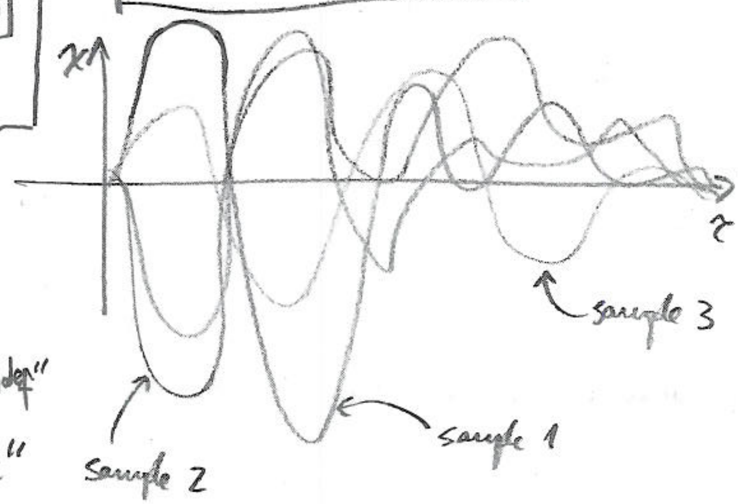
In QM, where $\langle O \rangle = \frac{1}{Z} \int \mathcal{D}[x(\tau)]\, e^{-S_E[x(\tau)]}\, O[x(\tau)]$

$$= \int \mathcal{D}[x(\tau)]\, O[x(\tau)]\, P[x(\tau)]$$

$$\boxed{P[x(\tau)] = \frac{e^{-S_E[x(\tau)]}}{Z}}$$

We can estimate

$$\boxed{\langle O \rangle \simeq \overline{O} = \frac{1}{N_{samples}} \sum_{n=1}^{N_{samples}} O[x_n(\tau)]}$$



Remember: This works only if P is well defined as a probability: $P[x] \geq 0$ "positive semidef"

$\int P[x]\, dx = 1$ "normalizable"

Main problem: How to generate configurations distributed according to $P[x(\tau)]$. → Sampling strategies.

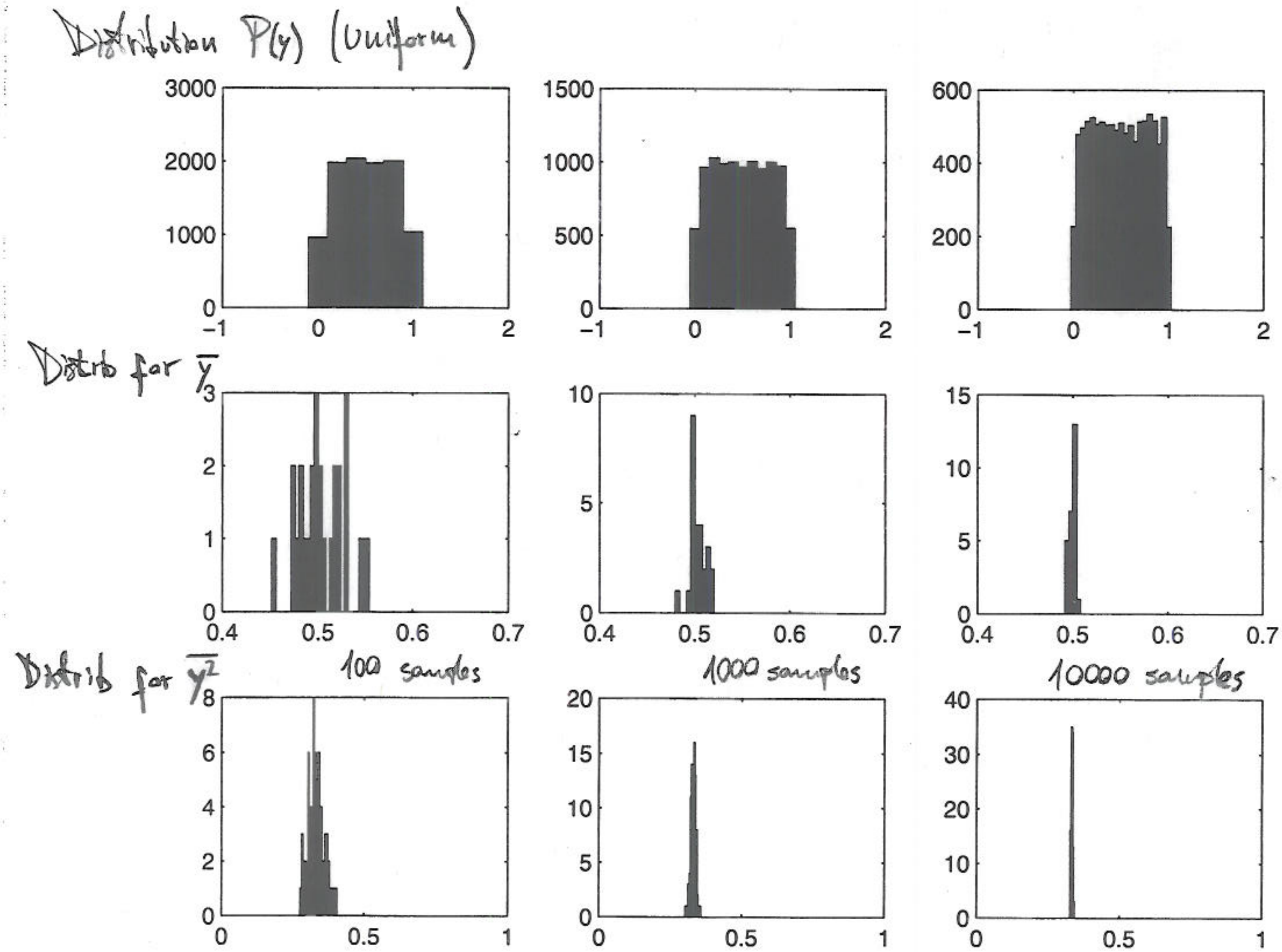
IV) Sampling strategies

- Heat-bath
- Metropolis ← typical for Ising model
- Molec. dynamics
- Hybrid

— Markov chain-based

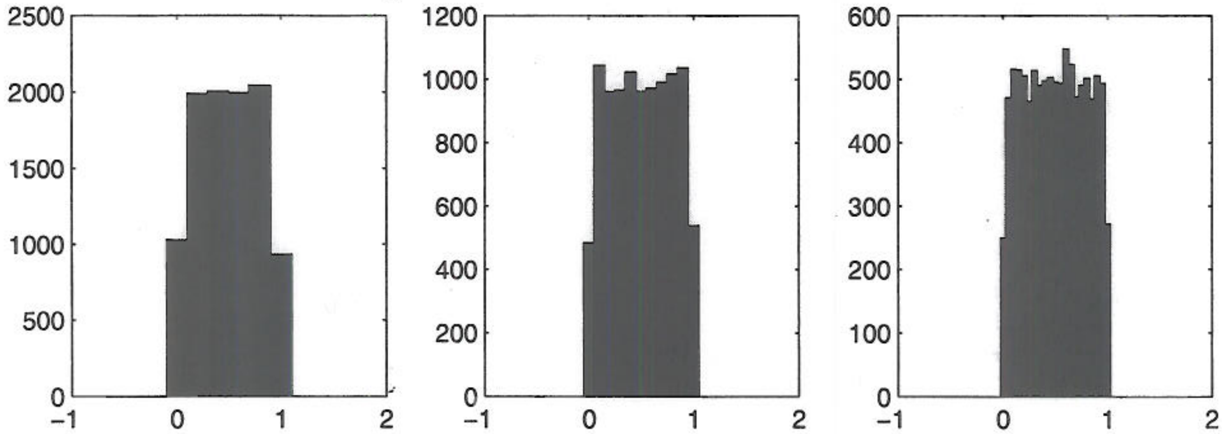
All of them can generate good samples if used properly.

- Equilibrated
- Uncorrelated

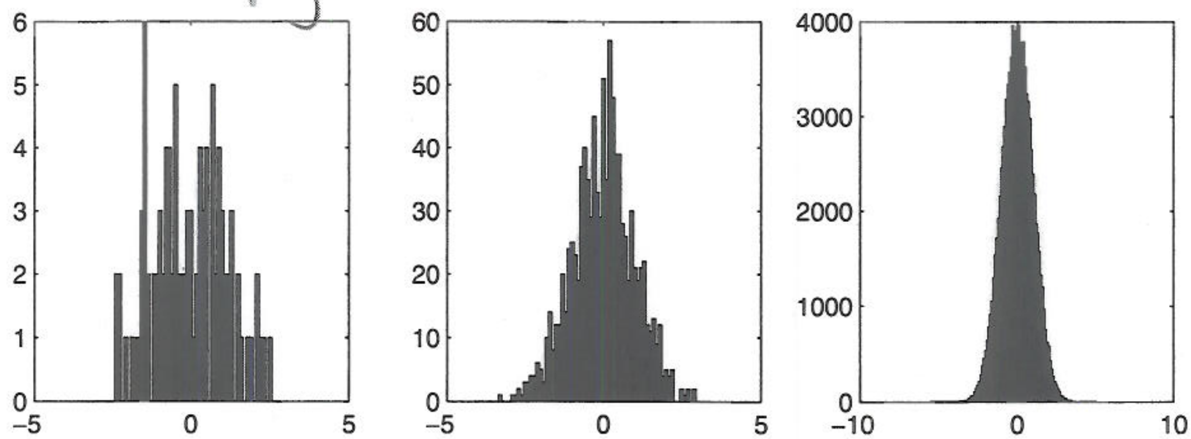


Distribution P(y) (Uniform)
Distrib for $\overline{y}$
Distrib for $\overline{y^2}$
100 samples
1000 samples
10000 samples

Uniform distribution sampling (10000 samples, variable bin size).



Gaussian distrib. sampling



100 samples

1000 samples

10000 samples