Probabilistic optimization in manufacturing

Simulated Annealing meets Set Packing

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https://github.com/michal-racko/pycon_pl_2025

What are Monte Carlo methods?

- Statistical techniques using random sampling
- Solve problems that are impossible or impractical to solve analytically
- Key principle: Use randomness to approximate deterministic results

Applications:

- Physics simulations
- Financial modeling
- Machine learning
- Engineering optimization

Starting at square one

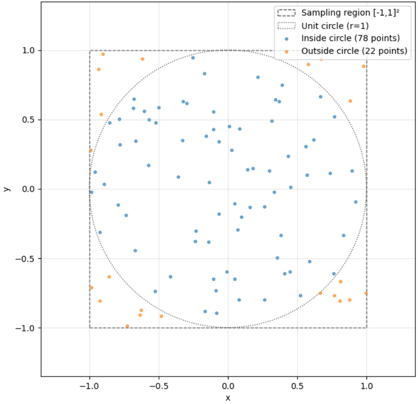
Value of π can be estimated using random sampling

Let's pretend π is an unknown constant which has to be estimated.

Geometric considerations

- Circle area: $A_{circle} = \pi$
- Square area: $A_{square} = 4$
- Ratio: $\frac{\pi}{4} = \frac{A_{circle}}{A_{square}}$

Therefore: $\pi = 4 \times \frac{A_{circle}}{A_{square}}$



Unit circle inscribed in square

Starting at square one

Value of π can be estimated using random sampling

Key Insight: All random points are uniformly distributed in the square

- Point (x, y) is inside circle if: $x^2 + y^2 \leq 1$
- Point (x, y) is outside circle if: $x^2 + y^2 > 1$

Therefore we can estimate

$$\pi \approx 4 \times \frac{\text{points inside circle}}{\text{total points}}$$

Starting at square one

Value of π can be estimated using random sampling

```
>>> import numpy as np
>>> class MonteCarloSamples:
...     def __init__(self, n_samples: int):
...         # Generate random points in [-1,1] x [-1,1]
...         self._samples = np.random.random((n_samples, 2)) * 2 - 1
...
...     def __len__(self) -> int:
...         return len(self._samples)
...
...     @property
...     def centre_distances(self) -> np.ndarray:
...         return np.sqrt((self._samples ** 2).sum(axis=1))
...
...     @property
...     def within_unit_circle(self) -> np.ndarray:
...         return self.centre_distances <= 1
...
...     @property
...     def pi_estimate(self) -> float:
...         return float(self.within_unit_circle.sum() / len(self) * 4)
...
>>> samples = MonteCarloSamples(100)
>>> print(samples.pi_estimate)
3.12
```

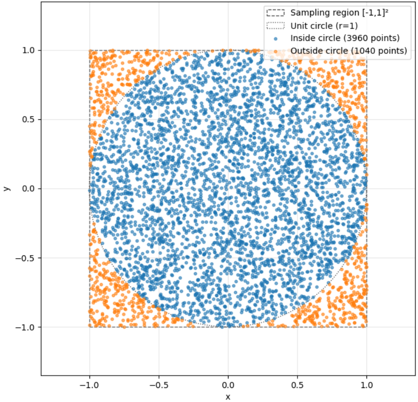
Starting at square one

Value of π can be estimated using random sampling

Adding more random samples improves precision

Geometric considerations

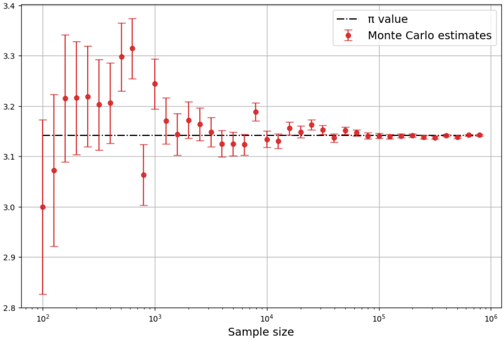
- 100 samples: $\pi \approx 3.12$
- 5,000 samples: $\pi \approx 3.1680$
- 10,000,000 samples: $\pi \approx 3.1408$



More random points drawn from the uniform distribution

Starting at square one

Value of π can be estimated using random sampling



Monte Carlo estimates converge to the true value as $N \to \infty$

Uncertainty estimation

- Our estimate follows: $X \sim \text{Binomial}(N, p)$
- $\text{Var}(\hat{\pi}) = 16 \cdot \frac{p(1-p)}{N}$
- Standard deviation: $\sigma \propto \frac{1}{\sqrt{N}}$

Starting at square one

Value of π can be estimated using random sampling

Estimating via Random Sampling: Random sampling can estimate quantities of interest when the experimental setup is well designed

Sample Size vs. Error: Estimation error decreases as sample size grows, although larger sample sizes increase computational complexity

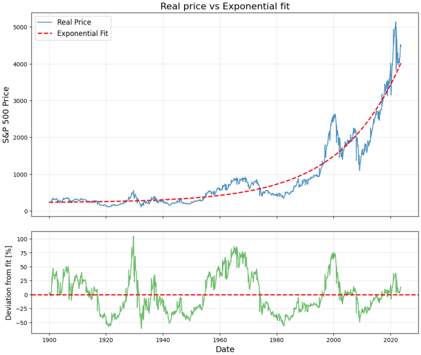
Quantifying Uncertainty: Uncertainty can be inferred using the properties of the probability distribution underlying the random samples

Let's divide and conquer

Decompose timeseries

- Exponential Trend: $P_\mathrm{e}(t) = a \cdot e^{bt} + c$
- Brownian motion: $\Delta P_\mathrm{b}(t) = \frac{P(t) - P_\mathrm{e}(t)}{P_\mathrm{e}(t)}$

$$P(t) = P_\mathrm{e}(t) \times (1 + \Delta P_\mathrm{b}(t))$$



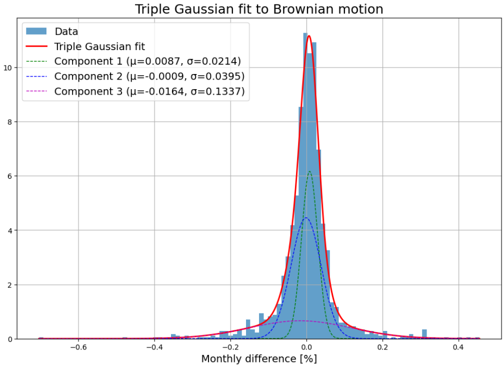
Exponential growth of S&P 500

S&P 500 price prediction

Monte Carlo can model complex or poorly understood processes

Triple Gaussian mixture:

$$f(x) = a_1 \cdot \mathcal{N}(\mu_1, \sigma_1^2) + a_2 \cdot \mathcal{N}(\mu_2, \sigma_2^2) + a_3 \cdot \mathcal{N}(\mu_3, \sigma_3^2)$$



Different regimes

- Normal market conditions
- Market stress/crashes
- Market euphoria/bubbles

S&P 500 price prediction

Monte Carlo can model complex or poorly understood processes

Now draw random samples from the fitted distribution

```
>>> import numpy as np
>>> N_SAMPLES = 10_000
>>> total_weight = a1 + a2 + a3
>>> component_choice = np.random.random(N_SAMPLES)
>>> samples = np.where(
...     component_choice < a1 / total_weight,
...     np.random.normal(mu1, sigma1, N_SAMPLES),
...     np.where(
...         component_choice < (a1 + a2) / total_weight,
...         np.random.normal(mu2, sigma2, N_SAMPLES),
...         np.random.normal(mu3, sigma3, N_SAMPLES)
...     )
... )
>>> samples
array([-0.00252675,  0.15553425,  0.0344586 , ...,  0.01754364,
       -0.01048925, -0.01011193], shape=(10000,))
```

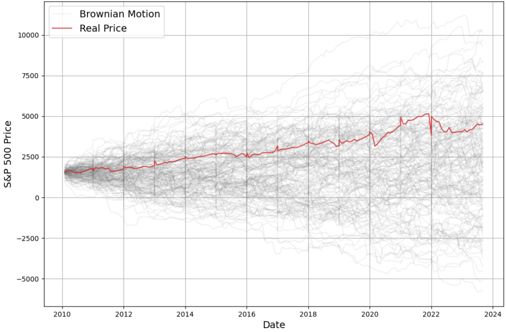
and repeat this for every timestep of our simulation. . .

S&P 500 price prediction

Monte Carlo can model complex or poorly understood processes

Many experiments

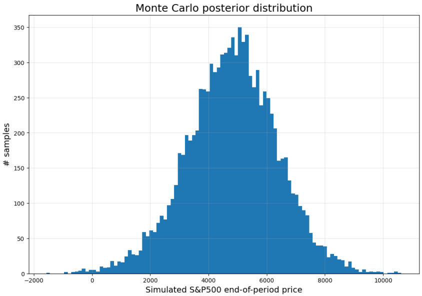
- Every simulated path represents an alternative reality following the same principles as our real data
- The more paths in a given region the more likely it is to occur
- Variance reduction techniques help focus on important regions



Simulated S&P 500 paths

S&P 500 price prediction

Monte Carlo can model complex or poorly understood processes



Monte Carlo posterior comprises results from all parallel experiments

Our simulation

- Gives probability estimates for future outcomes
- Past two years gets a Z-score of 1.0444
- While this model is rather simplistic it still provides useful insights

S&P 500 price prediction

Monte Carlo can model complex or poorly understood processes

Modeling with Monte Carlo: Complex or poorly understood processes can be modeled using random distributions, which Monte Carlo methods then leverage to simulate possible future outcomes

Assessing Future Outcomes: Posterior distributions allow us to estimate the likelihood of future outcomes, providing a powerful tool for assessing risks and opportunities

Statistical Weight Implementation: Variance reduction techniques allow our model to concentrate computational effort on the most important regions of the outcome space

Probabilistic optimization

Simulated Annealing escapes local optima

The Challenge: Roadtrip around Poland

Problem complexity

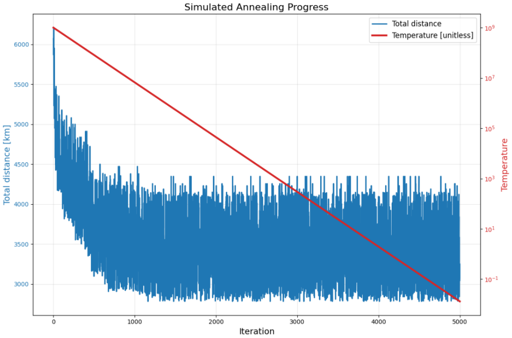
- NP-hard optimization problem
- $(n-1)!/2$ possible routes for n cities
- 21 cities $\rightarrow \sim 10^{18}$ combinations

Naive solution to TSP gets trapped in a local minimum

Probabilistic optimization
Simulated Annealing escapes local optima

Common for:

- Sheet metal production
- Quartz minerals
- Nuclear energy



Boltzmann Distribution:

$$P(E) \propto e^{-\frac{E}{k_B T}}$$

Simulated analogy:

$$P(\text{accept worse solution}) = e^{-\frac{\text{distance increase}}{T}}$$

Probabilistic optimization

Simulated Annealing escapes local optima

Algorithm

- **Exploration phase**
  high T $\Rightarrow$ most moves are accepted
- **Exploitation phase**
  low T $\Rightarrow$ only improvements are accepted

My implementation

Batch annealing plant optimization

Simulated annealing finds approximation to the optimal solution

Probabilistic optimization

Simulated Annealing escapes local optima

Monte Carlo in Optimization: Randomness enables exploration of solution spaces that deterministic algorithms cannot effectively navigate

Temperature Scheduling: Controlled cooling balances exploration (high temperature) with exploitation (low temperature) to find global optima

Real-world Impact: TSP principles apply to logistics, manufacturing, and many more. . .

Thank You!

I'm looking forward to answering your questions