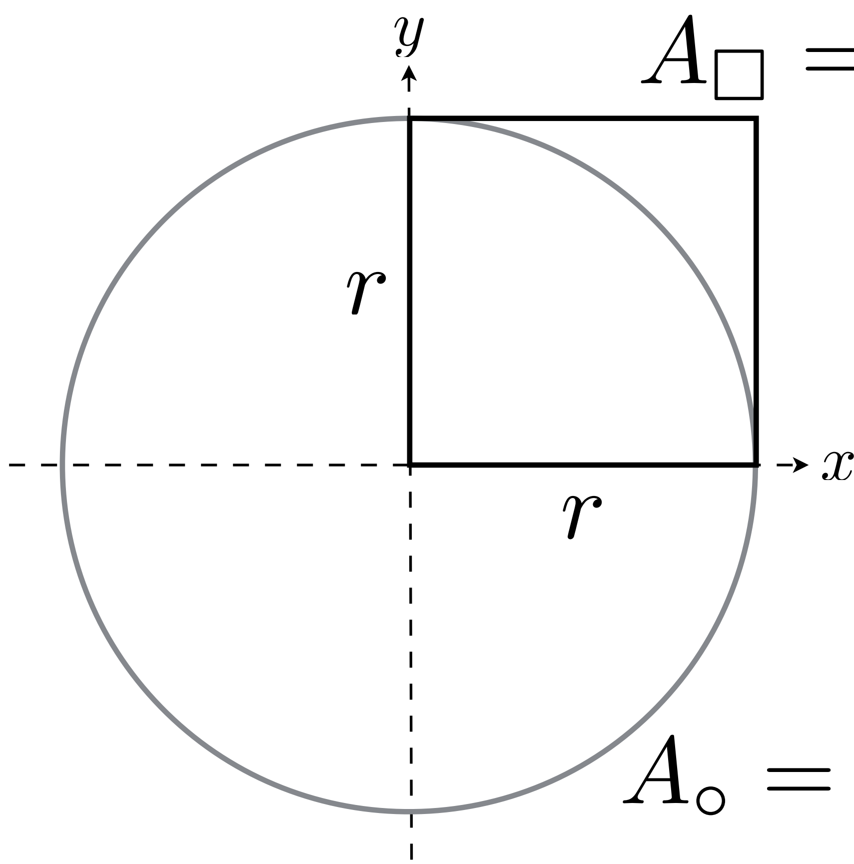
Computational Sciences Projektseminar

Markov chain Monte Carlo for particle-particle interactions

Recap: approximate π

$$A_\square = r^2$$



$$A_\circ = \pi r^2$$

$$\chi(x,y) = \begin{cases} 1, & x^2 + y^2 \leq r^2 \\ 0, & else \end{cases}$$

$$\frac{\frac{1}{4}A_\circ}{A_\square} \approx \frac{1}{N}\sum_{n=0}^{N-1}\chi(x_n, y_n)$$

$$\frac{\frac{1}{4}A_\circ}{A_\square} = \frac{\frac{1}{4}\pi r^2}{r^2} = \frac{\pi}{4}$$

$$(x_n, y_n) \in [0, r]^2 \; \forall n$$

`https://github.com/markovmodel/compsci-2017`

Sampling revisited: detailed balance

$$\pi(x)\, p(y|x) = \pi(y)\, p(x|y)$$

$$\begin{aligned}
\int_\Omega \mathrm{d}x\, \pi(x)\, p(y|x) &= \int_\Omega \mathrm{d}x\, \pi(y)\, p(x|y) \\
&= \pi(y) \int_\Omega \mathrm{d}x\, p(x|y) \\
&= \pi(y)
\end{aligned}$$

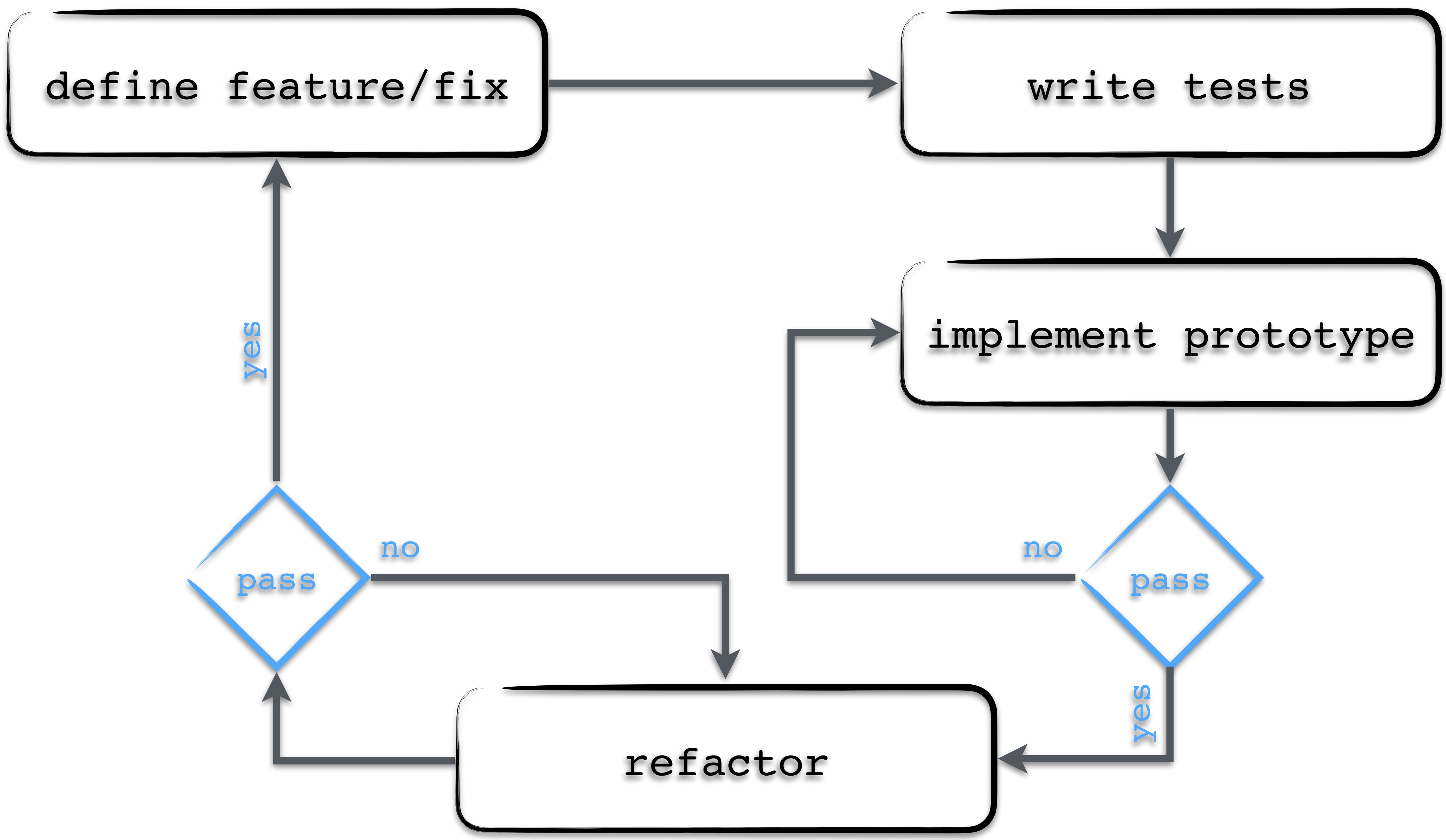
Sampling revisited: Metropolis Monte Carlo

$$x_{\mathrm{trial}} = x_{n-1} + \delta x$$

$$x_n = \begin{cases} x_{\mathrm{trial}}, & p < \mathbb{A}(x_{\mathrm{trial}}|x_{n-1}) \\ x_{n-1}, & \text{else} \end{cases}$$

$$\begin{aligned} \mathbb{A}(y|x) &= \min\left\{1, \frac{\pi(y)}{\pi(x)}\right\} \\ &= \min\left\{1, \frac{e^{-\beta\Phi(y)}}{e^{-\beta\Phi(x)}}\right\} \\ &= \min\left\{1, e^{\beta(\Phi(x)-\Phi(y))}\right\} \end{aligned}$$

Test-driven development (TDD)



Particle-particle interactions: Lennard-Jones

$$
\begin{aligned}
r_{ij} &= \|\mathbf{r}_i - \mathbf{r}_j\|_2 \\
\phi_{\mathrm{LJ}}(r) &= 4\epsilon\left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^6}{r^6}\right) \\
\Phi_{\mathrm{LJ}}(\mathbf{r}_1, \ldots, \mathbf{r}_N) &= \sum_{i<j} \phi_{\mathrm{LJ}}(r_{ij})
\end{aligned}
$$

- Pauli repulsion and van der Waals attraction
- very short-ranged
- easy to truncate