ALGORITHMIC PERSPECTIVE ON STRONGLY CORRELATED SYSTEMS

Lecture: Psi vs. Psi2

Fall 2015
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Psi vs Psi2

In our first quantum Monte Carlo code, we saw how to build your first quantum Monte Carlo code that 'sampled R with probability $|\Psi(R)|$'

We saw that this was good to get the energy but not so good for computing other observables.

Today, we'd like to do better. We'd like to figure out how to sample R with probability $|\Psi(R)|^2$

Two approaches:

1. Forward walking

2. Reptation

Let's start by recalling what we meant by 'sampling a basis element R with a given probability'

We have an algorithm where you hit a button and get a configuration R with probability P(R)…

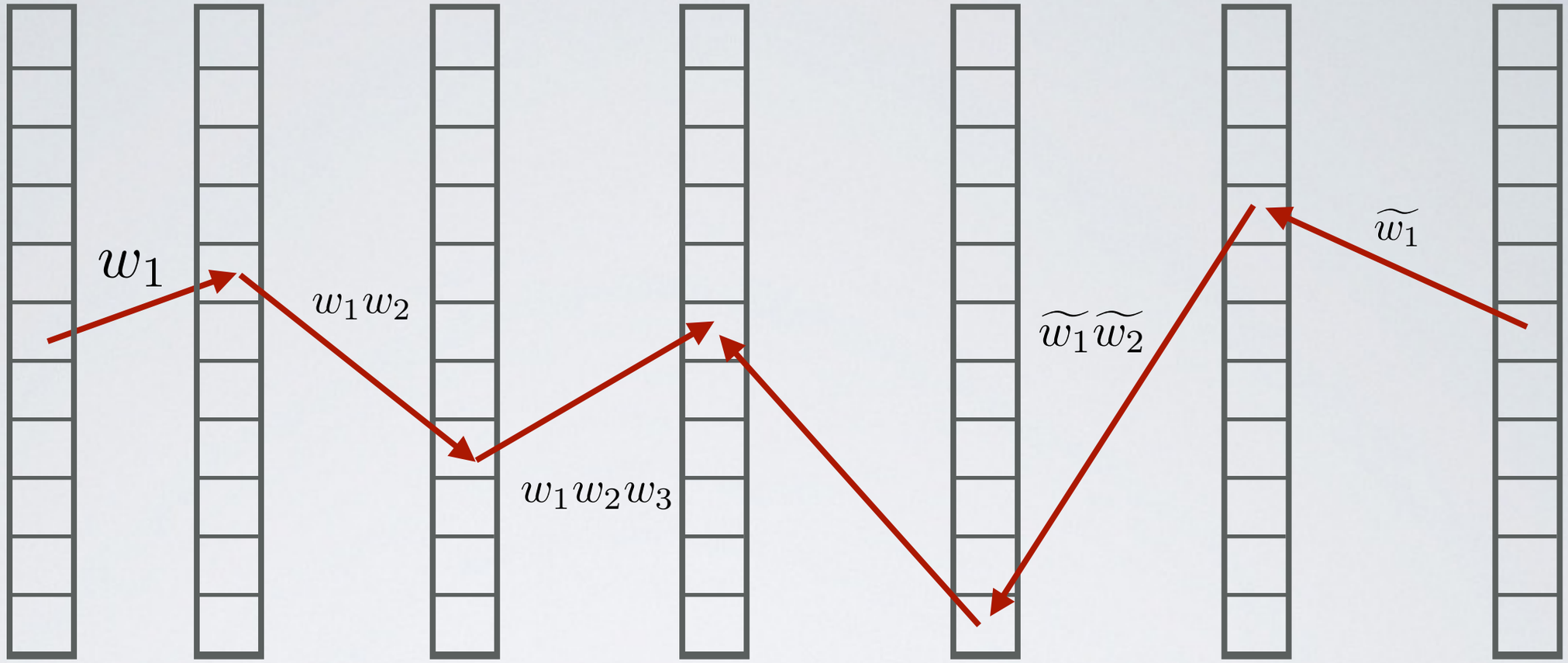
and that configuration comes with a weight w(R) …

with the property that $\Psi(R) \propto w(R)P(R)$

We'd like to make a small modification to this algorithm. We'd like to change it so that

$$|\Psi(R)|^2 \propto \widetilde{w(R)}P(R)$$

Q: How do we go about doing this?

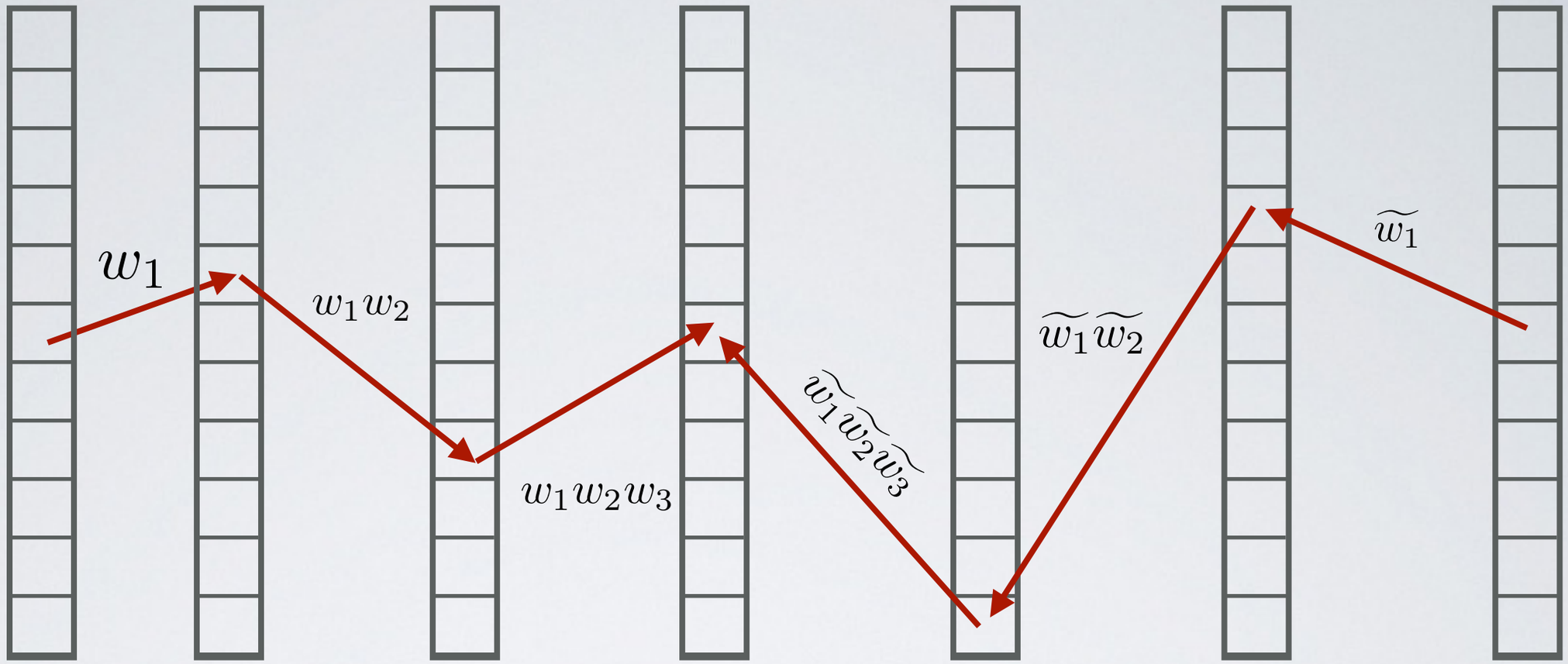


Q: Is this legal?

Q: Does this work?

Q: What about paths that don't collide?

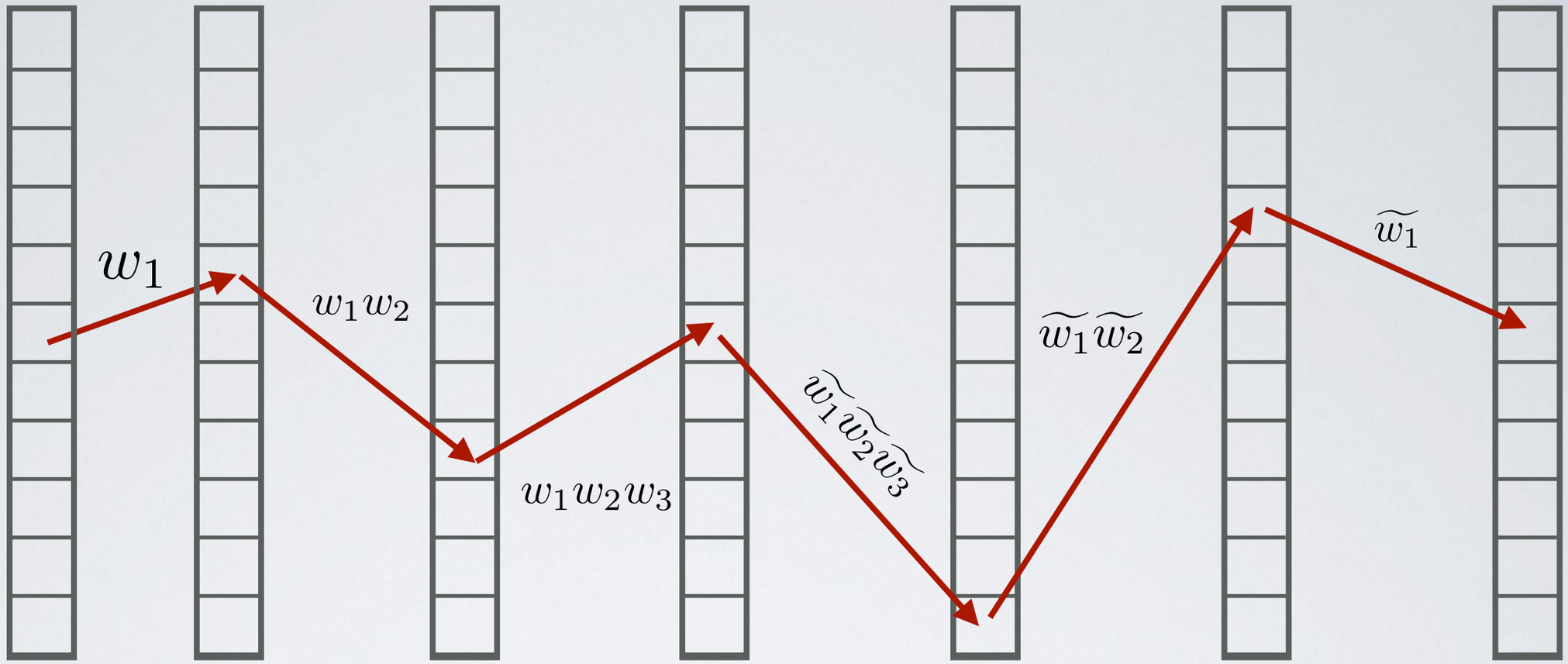
Q: Where are you measuring the observables?



At the end of the day, we have some probability of getting to R4 and some weight on R4 whose product should be (for this path) equal to….

$$\Psi(R_0)H(R_1,R_2)H(R_2,R_3)H(R_3,R_4)$$
$$\Psi(R_7)H(R_7,R_6)H(R_6,R_5)H(R_5,R_4)$$

Q: Can we arrange to get the (probability of being on R4) * (the weight we 'use' for R4) to be this for this path in some alternate way?

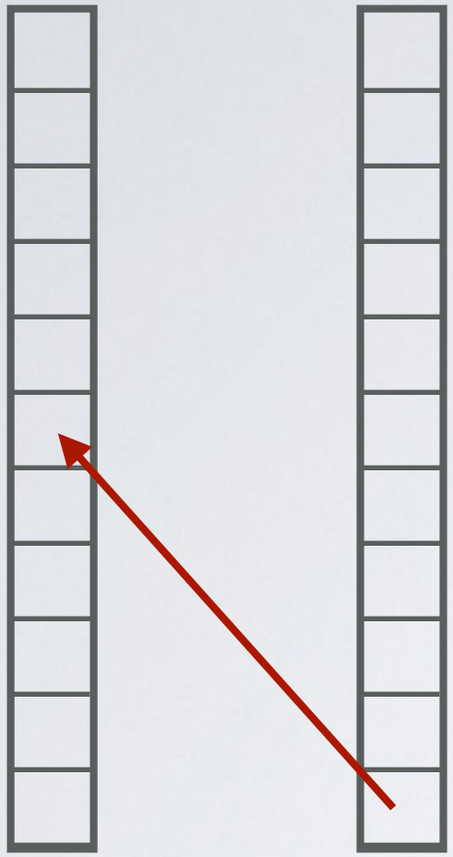


Q: Can we arrange to get the (probability of being on R4) * (the weight we 'use' for R4) to be this for this path in some alternate way?

Must multiply by $\Psi(R_7)$ when you reach the end.

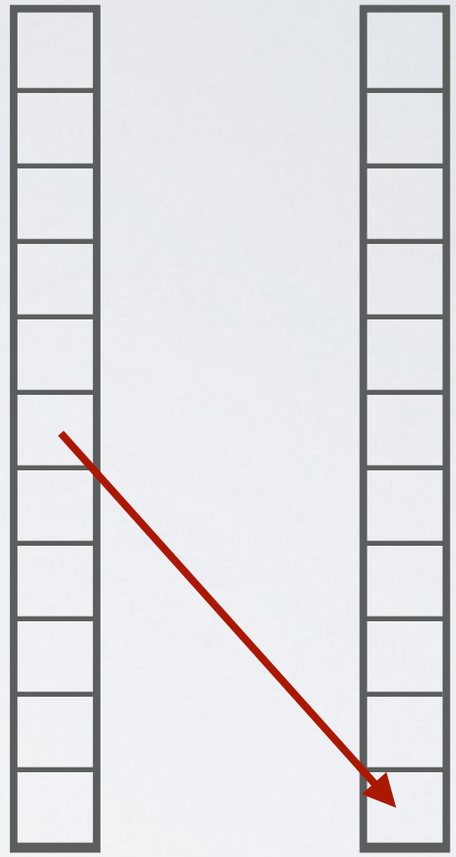
Measure on R4

A subtlety



$$\frac{G(R_{11}, R_6)}{\sum_i G(R_{11}, R_i)} \sum_i G(R_{11}, R_i)$$

P w



$$\frac{G(R_6, R_{11})}{\sum_i G(R_6, R_i)} \sum_i G(R_6, R_i)$$

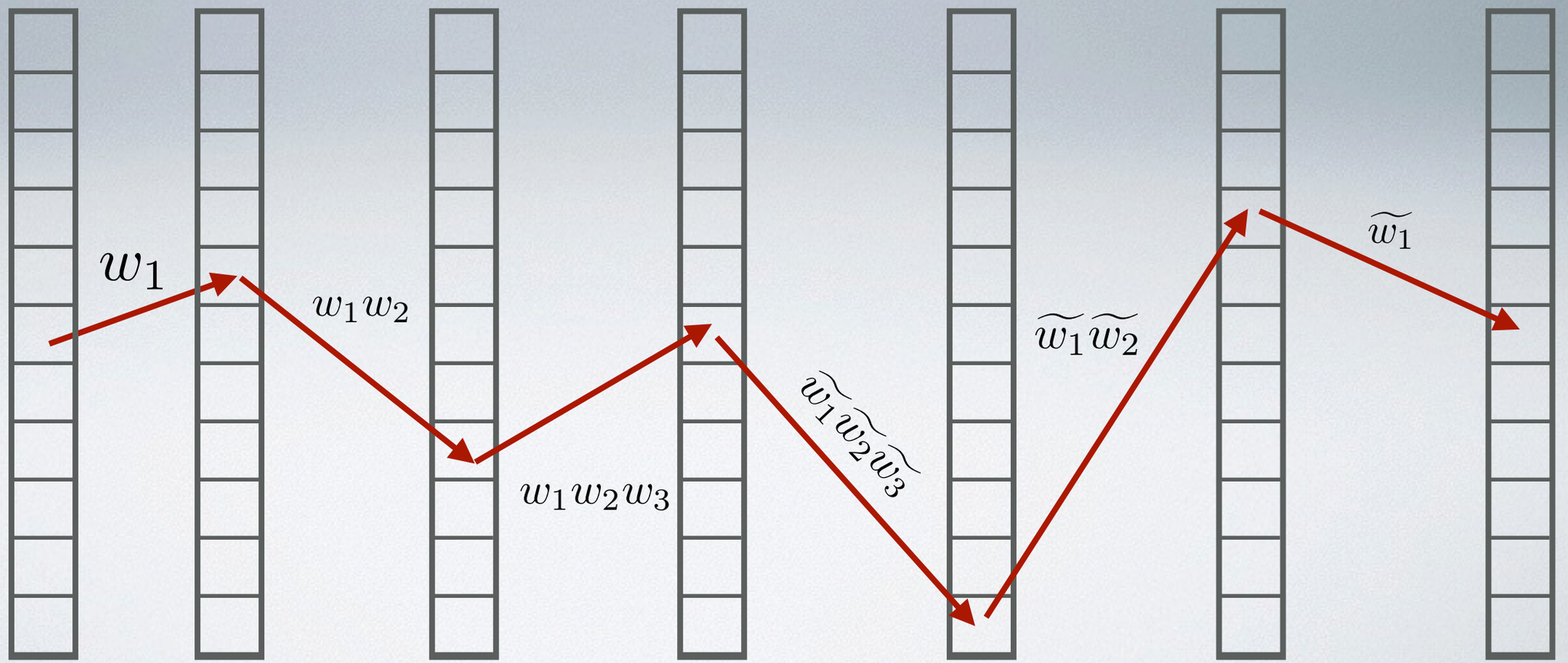
P w

These aren't the same…

Q: Does this completely solve our problem?

Q: Are there any downsides?

There are no free lunches…



We've learned about two 'types' of Monte Carlo…

* Markov Chain Monte Carlo (variational Monte Carlo)

* Projector Monte Carlo (matrix multiplication)

Can we actually use MCMC here somehow?

Currently: Stores the current "vector" in memory

New approach: store the entire path

…