Lecture 27: Physics-informed deep neural networks

Professor Ilias Bilionis

Sequential Monte Carlo

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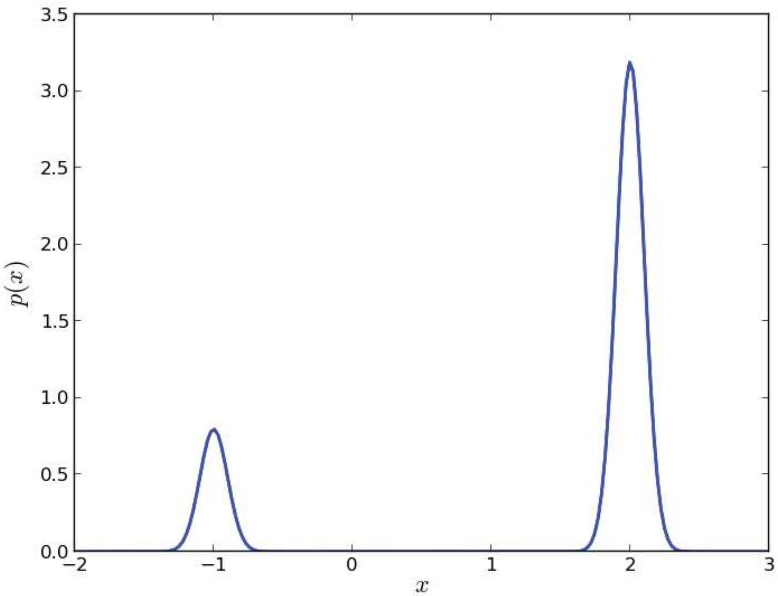
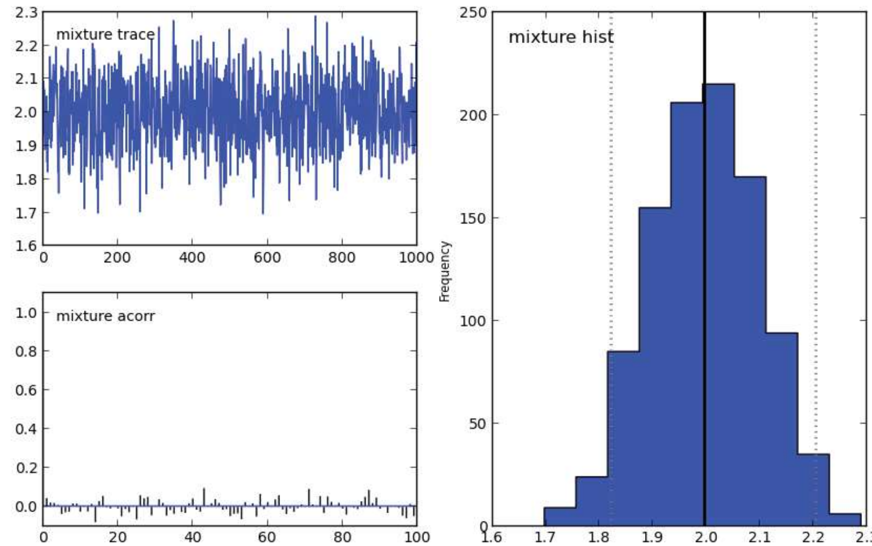
Limitations of MCMC

- Slow convergence.
- Trouble with multiple modes.
- Hard to calculate the normalization constant.

Example: Probability with two modes





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Bridging densities

Prior : $x \sim p(x)$

Likelihood : $y|x \sim p(y|x)$

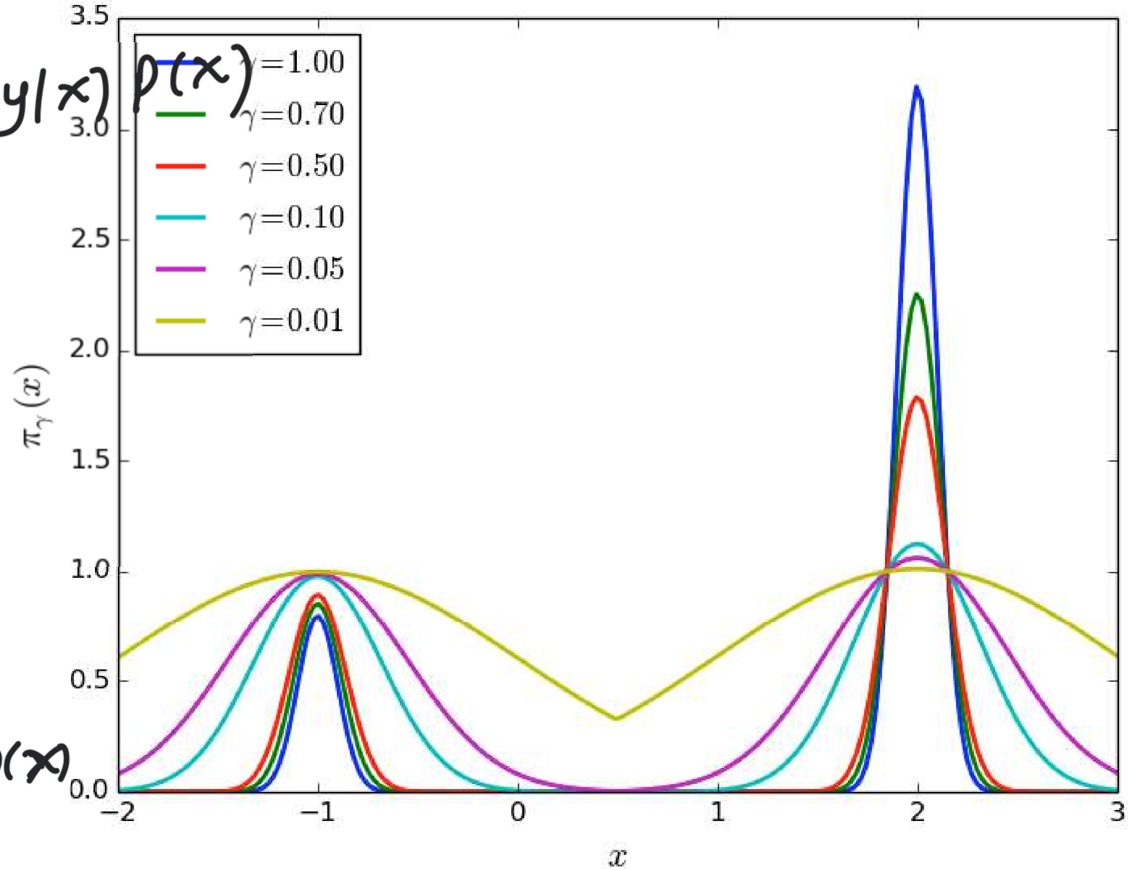
Posterior : $x|y \sim p(x|y) \propto p(y|x)\, p(x)$

IDEA : $0 \leq \gamma \leq 1$

$$\pi_\gamma(x) \propto [p(y|x)]^\gamma \, p(x)$$

$\gamma = 0$: $\pi_0(x) = p(x)$

$\gamma = 1$: $\pi_1(x) \propto p(y|x)\, p(x)$



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Sequential particle approximations

$N = \#$ of particles (samples)

$\gamma = 0$: $x_0^{(i)} \sim p(x)$, $w_0^{(i)} = \frac{1}{N}$, $\{(\underbrace{x_0^{(i)}}_{\text{particle}}, \underbrace{w_0^{(i)}}_{\text{weight}})\}_{i=1}^{N}$

$\downarrow$

γ : $\{(x_\gamma^{(i)}, w_\gamma^{(i)})\}_{i=1}^{N}$

- $w_\gamma^{(i)} = \dots$
- sample $x_\gamma^{(i)}$ w/ MCMC

$\downarrow$

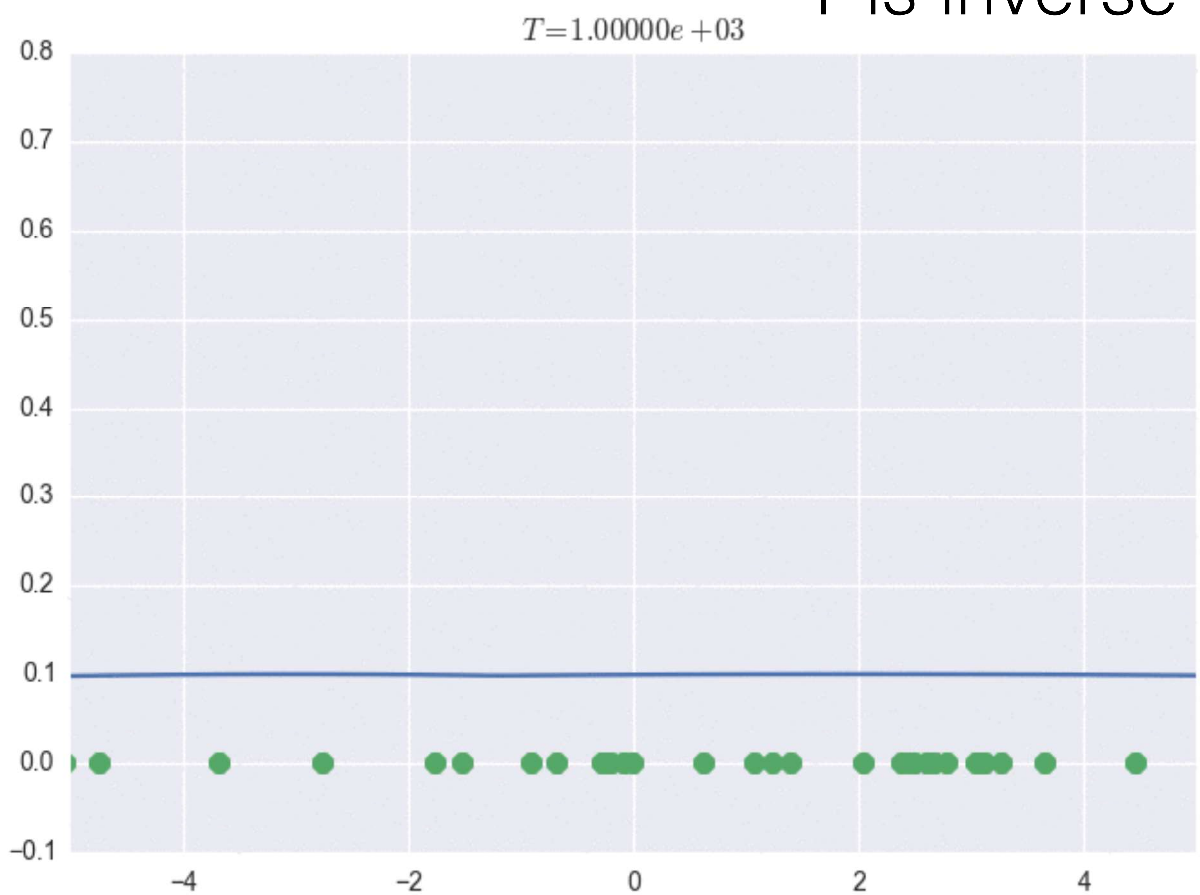
$\gamma = 1$: $\{(x_1^{(i)}, w_1^{(i)})\}$

$$\mathbb{E}[f(x) | y] \approx \sum_{i=1}^{N} w_1^{(i)} f(x_1^{(i)})$$

*Bilionis, I., et al. (2015). "Crop physiology calibration in the CLM." Geoscientific Model Development **8**(4): 1071-1083.*

Example

T is inverse gamma



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Estimating the normalization constant

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

$$Z = \int p(y|x)\,p(x)\,dx$$

If $p(x)$ is normalized, then SMC gives you a good estimate of Z.

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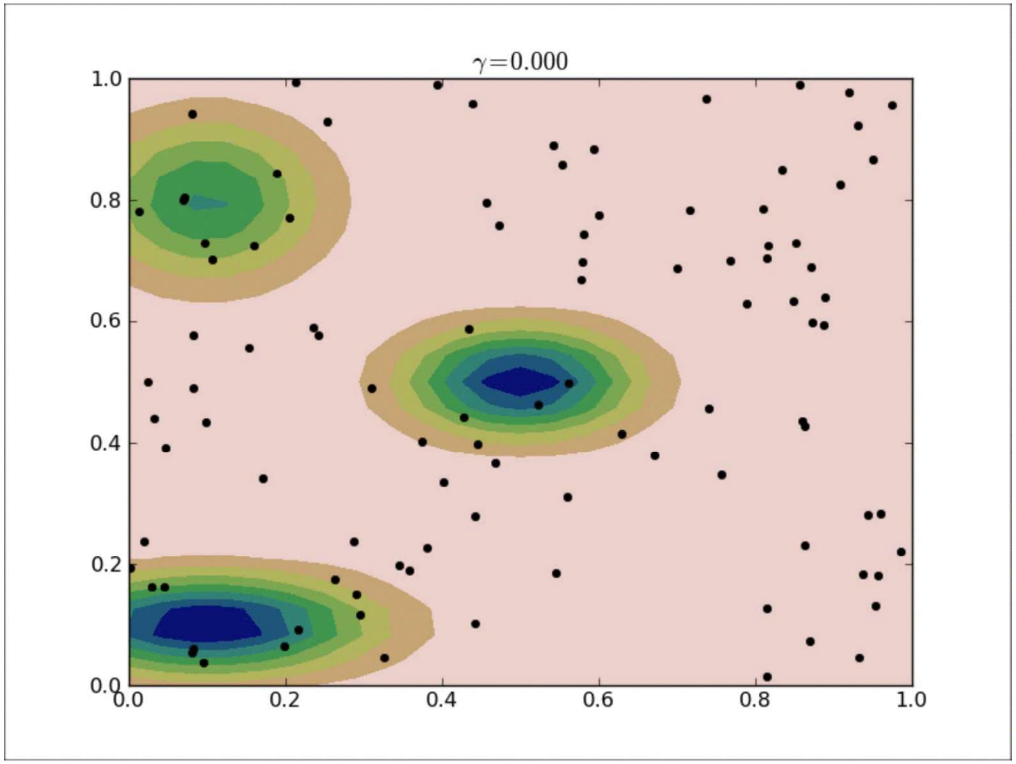
Resampling

- Some particle weights become too small.
- Every once in a while we can through them away and redistribute the weights.
- This is **resampling**.



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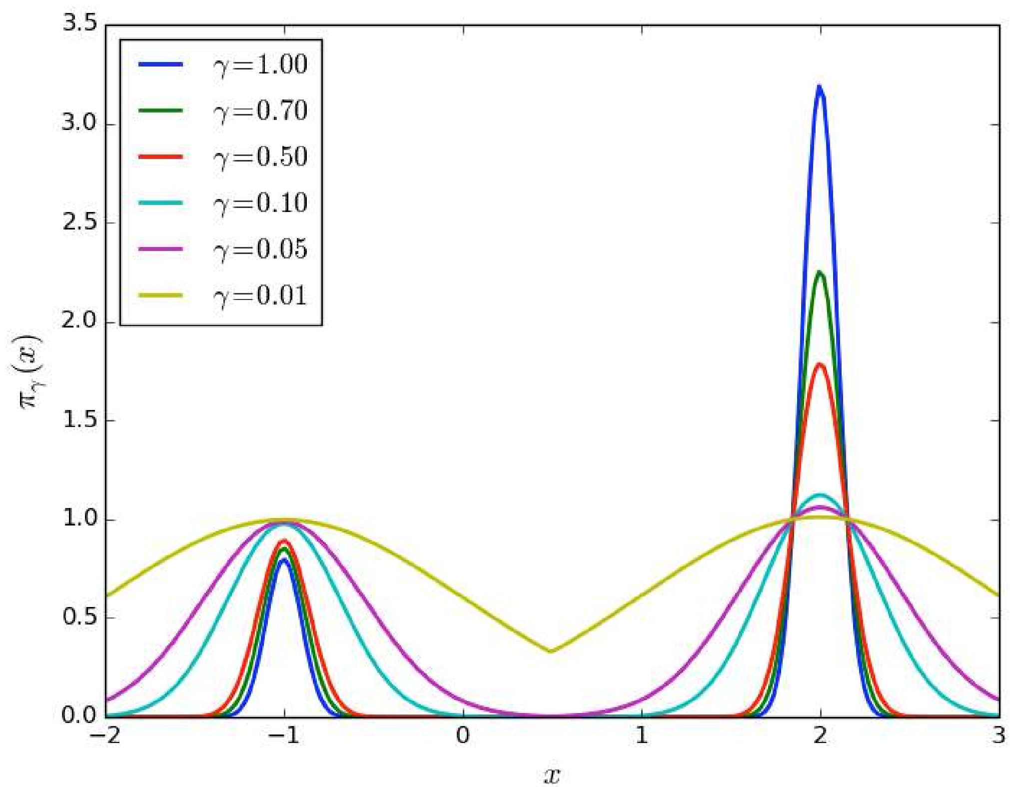
How fast should you change γ?

- You can just pick a fixed schedule.
- Or you can adaptively pick it.



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The complete SMC algorithm

- Build initial particle approximation (sample the prior).
- Find the next gamma.
- Resample if needed.
- Sample particle positions at new gamma starting from the old particles.