Monte-Carlo Estimation

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Setting: Computing expectations

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Predictions in a Bayesian model
"Average predictive distribution"

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Key idea

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- Compute expectations via statistical sampling:

$$\mathbb{E}[f(\boldsymbol{x})] = \int f(\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x} \approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)}), \quad \boldsymbol{x}^{(s)} \sim p(\boldsymbol{x})$$

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- Example: Making predictions in a supervised setting (e.g., Bayesian logistic regression with training set $\mathcal{D} = \{\boldsymbol{X}, \boldsymbol{y}\}$ at test input $\boldsymbol{x}_*$)

$$p(y_*|\boldsymbol{x}_*, \mathcal{D}) = \int p(y_*|\boldsymbol{\theta}, \boldsymbol{x}_*) \underbrace{p(\boldsymbol{\theta}|\mathcal{D})}_{\text{parameter posterior}} d\boldsymbol{\theta}$$

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Properties of Monte Carlo estimation

$$\mathbb{E}[f(\boldsymbol{x})] = \int f(\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x} \approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)}), \quad \boldsymbol{x}^{(s)} \sim p(\boldsymbol{x})$$

- Estimator is unbiased and asymptotically consistent, i.e.,

$$\lim_{S\to\infty} \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)}) = \mathbb{E}[f(\boldsymbol{x})] + \epsilon$$

- Error ϵ is normal (Gaussian) and its variance shrinks $\propto 1/S$, independent of the dimensionality

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- Sampling from simple distributions
  - Use libraries if the distribution has a “name”

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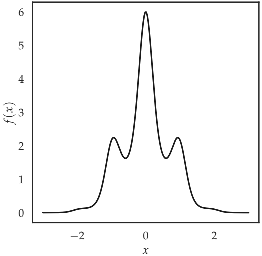
  ⏩ Use libraries if the distribution has a "name"
- Sampling from complicated distributions
  - Rejection sampling (does not scale to high dimensions)
  - Importance sampling (does not scale to high dimensions)
  - Markov chain Monte Carlo (MCMC) ⏩ Iain Murray's NeurIPS-2015 tutorial

Example



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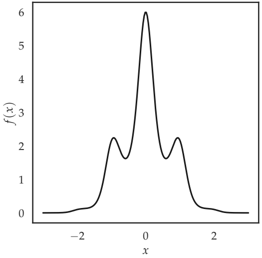

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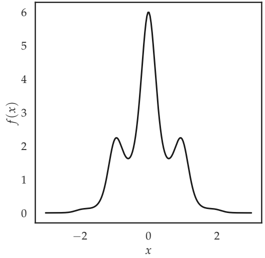

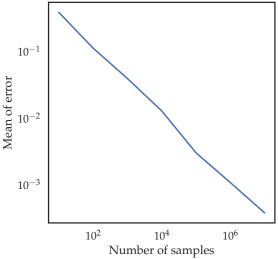

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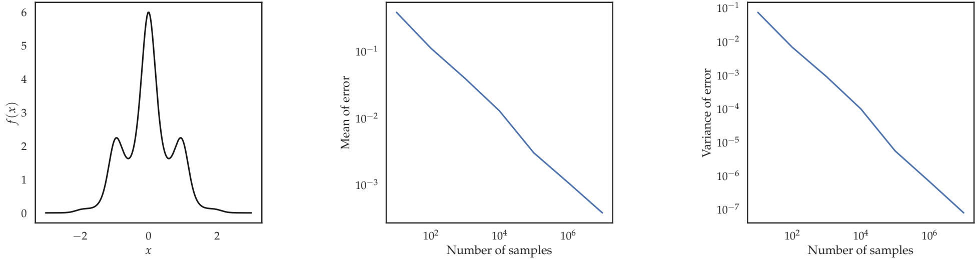

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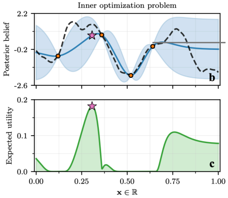
Some application areas

- Empirical risk minimization (Vapnik, 1991)
- Reinforcement learning (e.g., Sutton & Barto, 1998)
- Bayesian optimization
  (e.g., Snoek et al., 2012; Wilson et al., 2018)
- Variational deep learning
  (e.g., Rezende et al., 2014; Kingma & Welling, 2014)
- Probabilistic programming
  ⏩ Frank Wood's NeurIPS-2015 tutorial



From Wilson et al. (2018)

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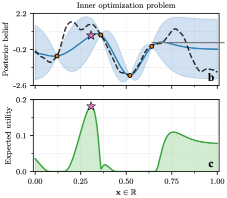
- High-energy physics (e.g., Buckley et al., 2011)
- Robotics (e.g., Dellaert et al., 1999)



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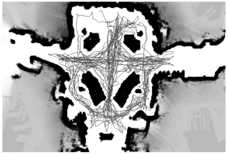


From Dellaert et al. (1999)

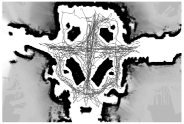
Considerations

$$\mathbb{E}[f(\boldsymbol{x})] \approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)}), \quad \boldsymbol{x}^{(s)} \sim p(\boldsymbol{x})$$

- Require many samples to get a good estimate of the value of the integral
- Design efficient samplers (computationally efficient, low variance)
- Function needs to be cheap to evaluate
- Good for learning, if we are just interested in an unbiased estimator
- Estimator does not take the locations of the samples into account
  - Could be problematic in small-sample regimes (O'Hagan, 1987)

Summary: Monte Carlo estimation

- Random numbers to compute expectations
- Estimator has nice properties
  (e.g., unbiased, asymptotically consistent)
- Scales to high dimensions
- General approach and straightforward
- Widely applicable
- Generating samples is the key challenge (not covered here)



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