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MCMC-driven (and optimization-based) adaptive importance samplers

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Outline

Importance Sampling: Basics

- Goal: $I = \int h(\mathbf{x})\widetilde{\pi}(\mathbf{x})d\mathbf{x}$
- **Importance sampling** (IS) approximates I if we cannot sample from $\widetilde{\pi}(\mathbf{x}) = \frac{\pi(\mathbf{x})}{Z}$ (or we do not want to)

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- Estimators of $I = \int h(\mathbf{x})\widetilde{\pi}(\mathbf{x})d\mathbf{x}$:

$$\widehat{I} = \frac{1}{NZ}\sum_{n=1}^{N} w_n h(\mathbf{x}_n), \quad \text{(UIS)}$$

$$\widetilde{I} = \sum_{n=1}^{N} \bar{w}_n h(\mathbf{x}_n), \quad \text{(SNIS)}$$

with $\bar{w}_n = \frac{w_n}{\sum_{i=1}^{N} w_i}$.

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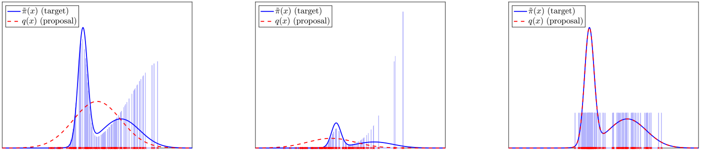
with $\bar{w}_n = \frac{w_n}{\sum_{i=1}^{N} w_i}$.
- Estimator of Z: $\widehat{Z} = \frac{1}{N}\sum_{n=1}^{N} w_n$

The variance in IS and the need of better proposals

- A good proposal $q(\mathbf{x})$ is key for the efficiency of IS.
- Variance of the UIS estimator:

$$\mathrm{Var}_{\widetilde{\pi}(\mathbf{x})}(\widehat{I}) = \frac{1}{N}\int \frac{h^2(\mathbf{x})\widetilde{\pi}^2(\mathbf{x})}{q(\mathbf{x})}d\mathbf{x} - \frac{I^2}{N}$$

- optimal UIS proposal: $q(\mathbf{x}) \propto |h(\mathbf{x})|\widetilde{\pi}(\mathbf{x})$
- for a generic $h(\mathbf{x})$, $q(\mathbf{x})$ should be as *close* as possible to $\widetilde{\pi}(\mathbf{x})$



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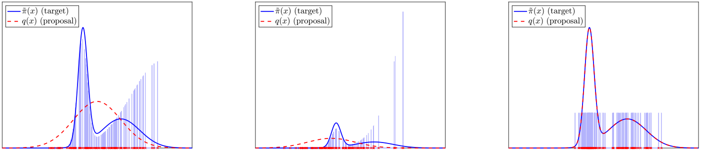

- Very difficult to find a good $q(\mathbf{x})$ a priori:
  - $\widetilde{\pi}(\mathbf{x})$ can be only evaluated (up to a normalizing constant)
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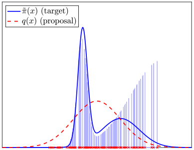

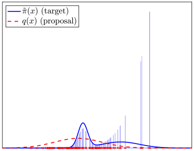

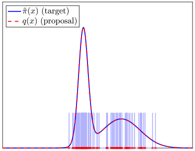

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  - $\widetilde{\pi}(\mathbf{x})$ can be only evaluated (up to a normalizing constant)
  - $\widetilde{\pi}(\mathbf{x})$ may be multimodal, skewed, heavy tailed
- Use **multiple** proposals (**MIS**) and **explore** the space (**AIS**).

Outline

Adaptive Importance Sampling: Basics

- A set of N proposals $\{q_{n,j}(\mathbf{x}|\boldsymbol{\theta}_{n,j})\}_{n=1}^{N}$ is adapted over $j = 1, ..., J$ iterations

$$\{q_{n,1}(\mathbf{x}|\boldsymbol{\theta}_{n,1})\}_{n=1}^{N} \rightarrow \{q_{n,2}(\mathbf{x}|\boldsymbol{\theta}_{n,2})\}_{n=1}^{N} \rightarrow ... \rightarrow \{q_{n,J}(\mathbf{x}|\boldsymbol{\theta}_{n,J})\}_{n=1}^{N}$$

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- AIS can be summarized to the process of adapting those parameters:

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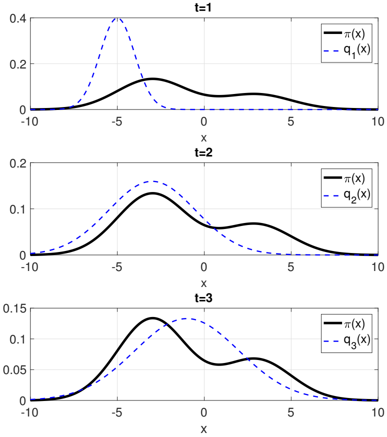

Adaptive Importance Sampling: Generic Algorithm

Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^{N}$, and initial parameters $\{\boldsymbol{\theta}_{n,1}\}_{n=1}^{N}$
For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate K samples per proposal

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\theta}_{n,j}), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

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Outputs: NKT weighted samples, $\{\mathbf{x}_{n,j}^{(k)}, w_{n,j}^{(k)}\}_{n=1,k=1,j=1}^{N,K,J}$

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Questions:

1. Weighting scheme?[2]

[2] V. E., L. Martino, D. Luengo, and M. F. Bugallo. "Generalized Multiple Importance Sampling". In: *Statistical Science* 34.1 (2019), pp. 129–155.

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1. Weighting scheme?
2. Adaptive procedure of $\boldsymbol{\theta}_{n,j}$?[3]

[3] M. F. Bugallo et al. "Adaptive importance sampling: The past, the present, and the future". In: *IEEE Signal Processing Magazine* 34.4 (2017), pp. 60–79.

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3. How do we build the estimators?

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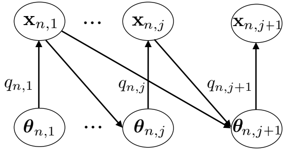
Classification of AIS methods

1. Adapt from previous samples via moment matching
2. Adapt from previous samples via resampling
3. Adapt from previous parameters (layered/hierarchical algorithms)

Classification of AIS methods (1)

1. Adapt from previous samples via moment matching

$$\{\mathbf{x}_{n,j}, w_{n,j}\}_{n=1}^{N} \xrightarrow{\text{moment matching}} \{\boldsymbol{\theta}_{n,j+1}\}_{n=1}^{N}$$



- M-PMC[5]: KL divergence minimization (MC estimate)
- APIS[6]: Multiple local approximations of target means
- **AMIS**[7]: Stochastic approximation of target moments
- CAIS[8]: Robust approximation of target moments

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[5] O. Cappé, R. Douc, A. Guillin, J. M. Marin, and C. P. Robert. "Adaptive importance sampling in general mixture classes". In: *Stat. Comput.* 18 (2008), pp. 447–459.

[6] L. Martino, V. E., D. Luengo, and J. Corander. "An adaptive population importance sampler: Learning from uncertainty". In: *IEEE Transactions on Signal Processing* 63.16 (2015), pp. 4422–4437.

[7] J. M. Cornuet, J. M. Marin, A. Mira, and C. P. Robert. "Adaptive Multiple Importance Sampling". In: *Scandinavian Journal of Statistics* 39.4 (Dec. 2012), pp. 798–812.

[8] Y. El-Laham, V. E., and M. F. Bugallo. "Robust covariance adaptation in adaptive importance sampling". In: *IEEE Signal Processing Letters* 25.7 (2018), pp. 1049–1053.

AMIS: Adaptive Multiple Importance Sampling (Cornuet et al., 2012)

Initialization: Choose J, K, q_1, $\boldsymbol{\mu}_1$ and $\mathbf{C}_1$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_1, \mathbf{C}_1)$
For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate K samples from q_j, i.e.,

$$\mathbf{x}_j^{(k)} \sim q_j(\mathbf{x}|\boldsymbol{\mu}_j, \mathbf{C}_j), \qquad k = 1, \ldots, K.$$

2. **Weighting:** (Re-)weight all current/past samples with a temporal mixture

$$w_\tau^{(k)} = \frac{\pi(\mathbf{x}_\tau^{(k)})}{\frac{1}{j}\sum_{i=1}^{j} q_i(\mathbf{x}_\tau^{(k)})}, \qquad k = 1, \ldots, K, \qquad \tau = 1, \ldots, j.$$

3. **Adaptation of the parameters:**[9][10] Update the mean and covariance with moment matching.

$$\{\mathbf{x}_\tau^{(k)}\}_{k=1,\tau=1}^{K,J} \xrightarrow{\text{mean estimate}} \{\boldsymbol{\mu}_{j+1}\},$$

$$\{\mathbf{x}_\tau^{(k)}\}_{k=1,\tau=1}^{K,J} \xrightarrow{\text{covariance estimate}} \{\mathbf{C}_{j+1}\},$$

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Classification of AIS methods (2)

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2. Adapt from previous samples via resampling:

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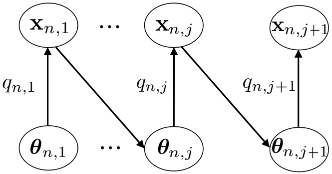

- PMC[11]
- **DM-PMC and variants**[12][13]

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[11] O. Cappé, A. Guillin, J. M. Marin, and C. P. Robert. "Population Monte Carlo". In: *Journal of Comp. and Graphical Statistics* 13.4 (2004), pp. 907–929.

[12] V. E., L. Martino, D. Luengo, and M. F. Bugallo. "Improving population Monte Carlo: Alternative weighting and resampling schemes". In: *Signal Processing* 131 (2017), pp. 77–91.

[13] V. E., L. Martino, D. Luengo, and M. F. Bugallo. "Population Monte Carlo schemes with reduced path degeneracy". In: *2017 IEEE 7th International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP)*. IEEE. 2017, pp. 1–5.

DM-PMC: Deterministic Mixture Population Monte Carlo (E. et al, 2017)

Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^{N}$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^{N}$ and $\{\mathbf{C}_n\}_{n=1}^{N}$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$

[14] V. E., L. Martino, D. Luengo, and M. F. Bugallo. "Improving population Monte Carlo: Alternative weighting and resampling schemes". In: *Signal Processing* 131 (2017), pp. 77–91.

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For $j = 1, \ldots, J$**:**

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2. **Weighting:** Weight the NK samples with the DM weights as

$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

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For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

2. **Weighting:** Weight the NK samples with the DM weights as

$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

3. **Adaptation of the parameters:**[14][15] Update the means via resampling
   - from the population of the NK samples to N location parameters

$$\{\mathbf{x}_{n,j}^{(k)}, w_{n,j}^{(k)}\}_{n=1,k=1}^{N,K} \xrightarrow{\text{Resampling}} \{\boldsymbol{\mu}_{n,j+1}\}_{n=1}^{N}$$

Outputs: NKJ weighted samples, $\{\mathbf{x}_{n,j}^{(k)}, w_{n,j}^{(k)}\}_{n=1,k=1,j=1}^{N,K,J}$

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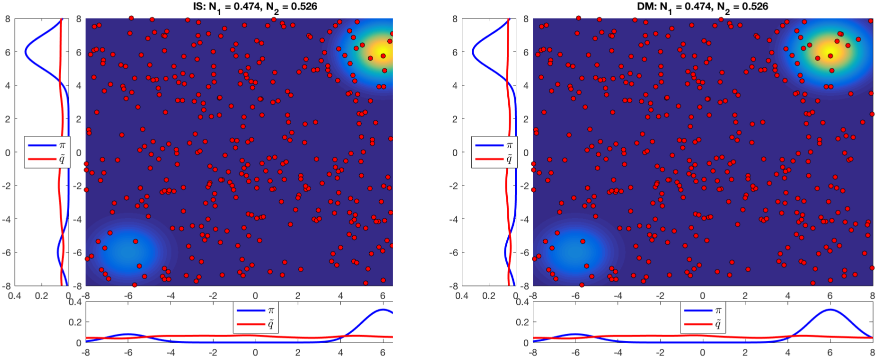
[14] V. E., L. Martino, D. Luengo, and M. F. Bugallo. "Improving population Monte Carlo: Alternative weighting and resampling schemes". In: *Signal Processing* 131 (2017), pp. 77–91.

[15] V. E., L. Martino, D. Luengo, and M. F. Bugallo. "Population Monte Carlo schemes with reduced path degeneracy". In: *2017 IEEE 7th International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP)*. IEEE. 2017, pp. 1–5.

DM-PMC: DM weights in resampling (iteration $j = 1$)

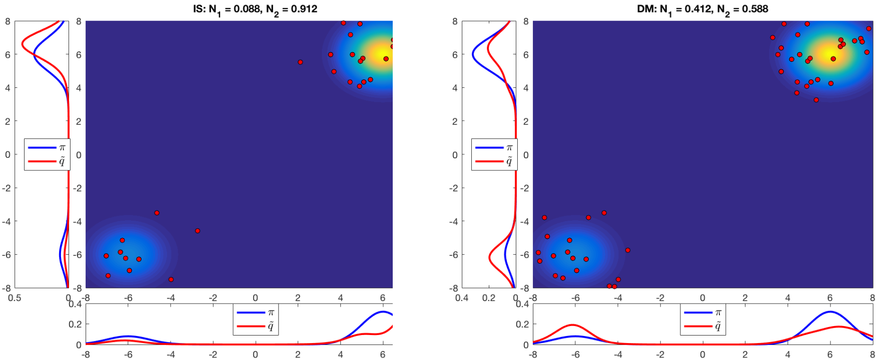


(a) Standard IS weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{q_{n,j}(\mathbf{x}_{n,j})}$.

(b) DM weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j})}$.

Figure: The red circles represent the means $\boldsymbol{\mu}_{n,j}$ of the IS proposals ($N = 500$) at iteration $j = 1$. Covariance of IS proposal $\mathbf{C}_n = \sigma_0^2 \mathbf{I}$, with $\sigma_0^2 = 0.5$.

DM-PMC: DM weights in resampling (iteration $j = 2$)

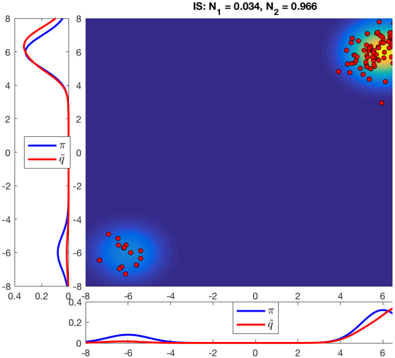


(a) Standard IS weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{q_{n,j}(\mathbf{x}_{n,j})}$.

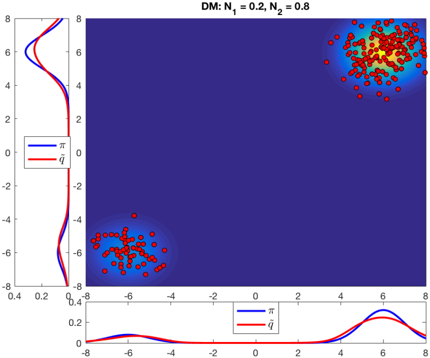
(b) DM weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j})}$.

Figure: The red circles represent the means $\boldsymbol{\mu}_{n,j}$ of the IS proposals ($N = 500$) at iteration $j = 2$. Covariance of IS proposal $\mathbf{C}_n = \sigma_0^2 \mathbf{I}$, with $\sigma_0^2 = 0.5$.

DM-PMC: DM weights in resampling (iteration $j = 3$)



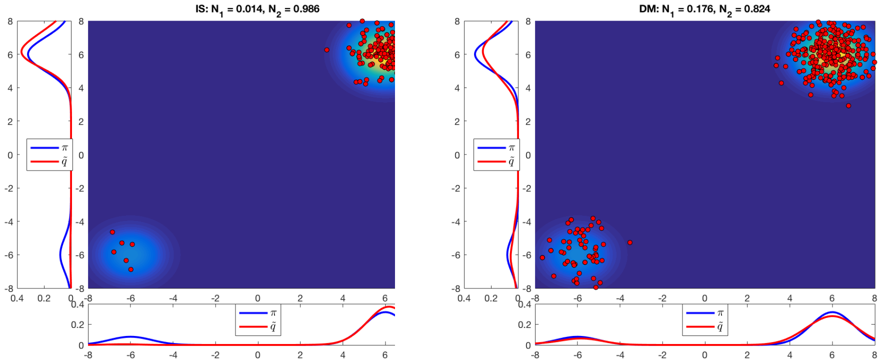
(a) Standard IS weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{q_{n,j}(\mathbf{x}_{n,j})}$.



(b) DM weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j})}$.

Figure: The red circles represent the means $\boldsymbol{\mu}_{n,j}$ of the IS proposals ($N = 500$) at iteration $j = 3$. Covariance of IS proposal $\mathbf{C}_n = \sigma_0^2\mathbf{I}$, with $\sigma_0^2 = 0.5$.

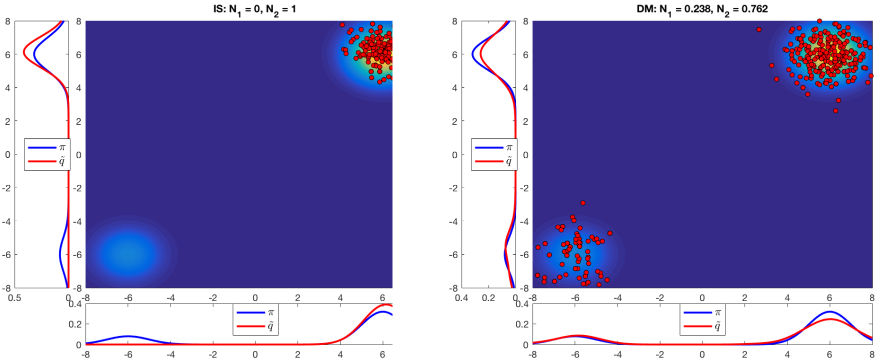
DM-PMC: DM weights in resampling (iteration $j = 4$)



(a) Standard IS weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{q_{n,j}(\mathbf{x}_{n,j})}$. (b) DM weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j})}$.

Figure: The red circles represent the means $\boldsymbol{\mu}_{n,j}$ of the IS proposals ($N = 500$) at iteration $j = 4$. Covariance of IS proposal $\mathbf{C}_n = \sigma_0^2\mathbf{I}$, with $\sigma_0^2 = 0.5$.

DM-PMC: DM weights in resampling (iteration $j = 5$)

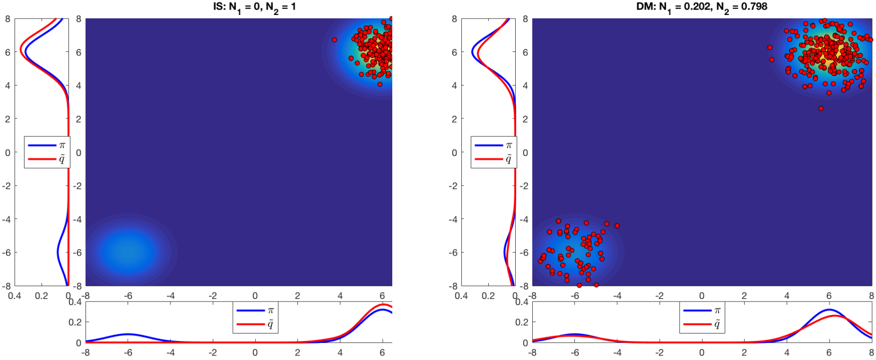


(a) Standard IS weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{q_{n,j}(\mathbf{x}_{n,j})}$.

(b) DM weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j})}$.

Figure: The red circles represent the means $\boldsymbol{\mu}_{n,j}$ of the IS proposals ($N = 500$) at iteration $j = 5$. Covariance of IS proposal $\mathbf{C}_n = \sigma_0^2\mathbf{I}$, with $\sigma_0^2 = 0.5$.

DM-PMC: DM weights in resampling (iteration $j = 6$)



(a) Standard IS weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{q_{n,j}(\mathbf{x}_{n,j})}$.

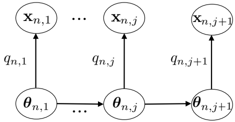
(b) DM weights $w_{n,j} = \frac{\pi(\mathbf{x}_{n,j})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j})}$.

Figure: The red circles represent the means $\boldsymbol{\mu}_{n,j}$ of the IS proposals ($N = 500$) at iteration $j = 6$. Covariance of IS proposal $\mathbf{C}_n = \sigma_0^2\mathbf{I}$, with $\sigma_0^2 = 0.5$.

Outline

Classification of AIS methods (3)

3. Adapt from previous parameters (layered/hierarchical algorithms)



- GAPIS[16]: gradient updates
- LAIS[17]: location parameters sampled via MCMC on $\widetilde{\pi}$
- O-PMC[18]: langevin dynamics and second-order information
- GRAMIS[19]: first and second order information of the target
- Purely optimization-based: variational inference[20][21], χ^2-div min.[22]

[16] V. E., L. Martino, D. Luengo, and J. Corander. "A gradient adaptive population importance sampler". In: *IEEE ICASSP*. IEEE. 2015, pp. 4075–4079.

[17] L. Martino, V. E., D. Luengo, and J. Corander. "Layered adaptive importance sampling". In: *Statistics and Computing* 27 (2017), pp. 599–623.

[18] V. E. and E. Chouzenoux. "Optimized population monte carlo". In: *IEEE Transactions on Signal Processing* 70 (2022), pp. 2489–2501.

[19] V. E., E. Chouzenoux, Ö. D. Akyildiz, and L. Martino. "Gradient-based Adaptive Importance Samplers". In: *Journal of the Franklin Institute (to appear in)* (2023).

[20] Y. El-Laham, P. M. Djurić, and M. F. Bugallo. "A variational adaptive population importance sampler". In: *IEEE ICASSP*. IEEE. 2019, pp. 5052–5056.

[21] G. Jerfel et al. "Variational refinement for importance sampling using the forward kullback-leibler divergence". In: *Uncertainty in Artificial Intelligence*. PMLR. 2021, pp. 1819–1829.

[22] E. K. Ryu and S. P. Boyd. "Adaptive importance sampling via stochastic convex programming". In: *arXiv preprint arXiv:1412.4845* (2014).

LAIS: Layered Adaptive Importance Sampling (Martino et al., 2017)

Initialization: Choose J, N, K, $\{q_{n,1}(\boldsymbol{\theta}_{n,1})\}_{n=1}^{N}$, $\boldsymbol{\theta}_{n,1} = [\boldsymbol{\mu}_{n,1}\ \mathbf{C}_n]$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$

[23] L. Martino, V. E., D. Luengo, and J. Corander. "Layered adaptive importance sampling". In: *Statistics and Computing* 27 (2017), pp. 599–623.

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Initialization: Choose J, N, K, $\{q_{n,1}(\boldsymbol{\theta}_{n,1})\}_{n=1}^{N}$, $\boldsymbol{\theta}_{n,1} = [\boldsymbol{\mu}_{n,1}\ \mathbf{C}_n]$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$
For $j = 1, \ldots, J$:

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

[23] L. Martino, V. E., D. Luengo, and J. Corander. "Layered adaptive importance sampling". In: *Statistics and Computing* 27 (2017), pp. 599–623.

LAIS: Layered Adaptive Importance Sampling (Martino et al., 2017)

Initialization: Choose J, N, K, $\{q_{n,1}(\boldsymbol{\theta}_{n,1})\}_{n=1}^{N}$, $\boldsymbol{\theta}_{n,1} = [\boldsymbol{\mu}_{n,1}\ \mathbf{C}_n]$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$
For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as
$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$
2. **Weighting:** Weight the NK samples with DM weights as
$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

[23] L. Martino, V. E., D. Luengo, and J. Corander. "Layered adaptive importance sampling". In: *Statistics and Computing* 27 (2017), pp. 599–623.

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Initialization: Choose J, N, K, $\{q_{n,1}(\boldsymbol{\theta}_{n,1})\}_{n=1}^{N}$, $\boldsymbol{\theta}_{n,1} = [\boldsymbol{\mu}_{n,1}\ \mathbf{C}_n]$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$

For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

2. **Weighting:** Weight the NK samples with DM weights as

$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

3. **Adaptation of the parameters:**[23] Update the means with one/several independent/dependent MCMC steps (upper layer)

$$\{\boldsymbol{\mu}_{n,j}\}_{n=1}^{N} \xrightarrow{\text{MCMC on } \tilde{\pi}} \{\boldsymbol{\mu}_{n,j+1}\}_{n=1}^{N},$$

Outputs: NKJ weighted samples, $\{\mathbf{x}_{n,j}^{(k)}, w_{n,j}^{(k)}\}_{n=1,k=1,j=1}^{N,K,J}$

[23] L. Martino, V. E., D. Luengo, and J. Corander. "Layered adaptive importance sampling". In: *Statistics and Computing* 27 (2017), pp. 599–623.

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Initialization: Choose J, N, K, $\{q_{n,1}(\boldsymbol{\theta}_{n,1})\}_{n=1}^{N}$, $\boldsymbol{\theta}_{n,1} = [\boldsymbol{\mu}_{n,1}\ \mathbf{C}_n]$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$

For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as
$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$
2. **Weighting:** Weight the NK samples with DM weights as
$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$
3. **Adaptation of the parameters:**[23] Update the means with one/several independent/dependent MCMC steps (upper layer)
$$\{\boldsymbol{\mu}_{n,j}\}_{n=1}^{N} \xrightarrow{\text{MCMC on } \tilde{\pi}} \{\boldsymbol{\mu}_{n,j+1}\}_{n=1}^{N},$$

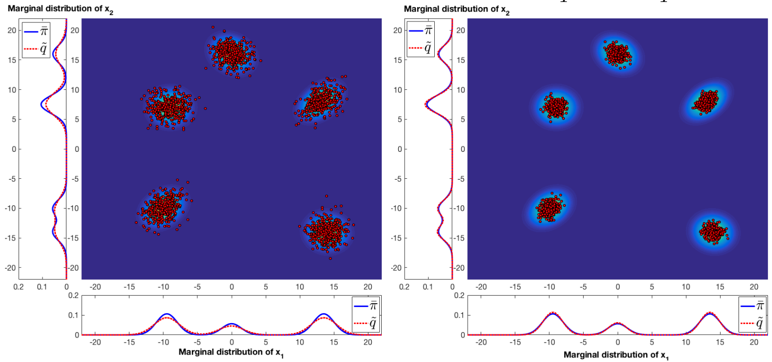
Outputs: NKJ weighted samples, $\{\mathbf{x}_{n,j}^{(k)}, w_{n,j}^{(k)}\}_{n=1,k=1,j=1}^{N,K,J}$

- LAIS can be seen as a mixture sampling from a KDE of $\tilde{\pi}$

[23] L. Martino, V. E., D. Luengo, and J. Corander. "Layered adaptive importance sampling". In: *Statistics and Computing* 27 (2017), pp. 599–623.

LAIS and AT-LAIS

- Anti-tempered LAIS (AT-LAIS)[24] runs the MCMC on $\tilde{\pi}^{\beta}$, $\beta > 1$, so the stationary distribution of the AIS samples is closer to $\tilde{\pi}$.
  - The red circles represent the means $\boldsymbol{\mu}$ of the IS proposals ($N = 2000$) in the last iteration. Covariance of IS proposal $\mathbf{C} = \sigma_T^2 \mathbf{I}$, with $\sigma_T^2 = 1$.



(a) LAIS ($\beta = 1$) (b) AT-LAIS ($\beta = 4$)

[24] L. Martino, V. E., and D. Luengo. "Anti-tempered layered adaptive importance sampling". In: *2017 22nd International Conference on Digital Signal Processing (DSP)*. IEEE. 2017, pp. 1–5.

[25] A. Mousavi, R. Monsefi, and V. E. "Hamiltonian adaptive importance sampling". In: *IEEE Signal Processing Letters* 28 (2021), pp. 713–717.

LAIS and AT-LAIS

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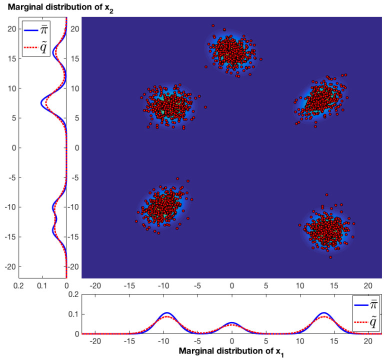
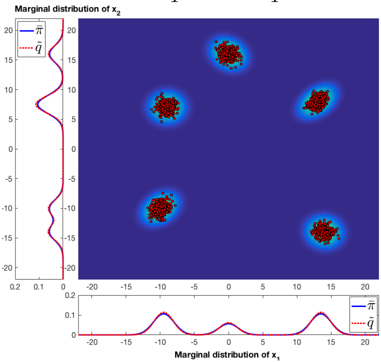


(c) LAIS ($\beta = 1$)



(d) AT-LAIS ($\beta = 4$)

- Hamiltonian AIS (HAIS) version[25]

[24] L. Martino, V. E., and D. Luengo. "Anti-tempered layered adaptive importance sampling". In: *2017 22nd International Conference on Digital Signal Processing (DSP)*. IEEE. 2017, pp. 1–5.

[25] A. Mousavi, R. Monsefi, and V. E. "Hamiltonian adaptive importance sampling". In: *IEEE Signal Processing Letters* 28 (2021), pp. 713–717.

O-PMC: Optimized Population Monte Carlo (E. and Chouzenoux, 2022)

Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^{N}$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^{N}$ and $\{\mathbf{C}_n\}_{n=1}^{N}$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$

[26] V. E. and E. Chouzenoux. "Optimized population monte carlo". In: *IEEE Transactions on Signal Processing* 70 (2022), pp. 2489–2501.

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Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^{N}$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^{N}$ and $\{\mathbf{C}_n\}_{n=1}^{N}$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$
For $j = 1, \dots, J$**:**

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \dots, K, \qquad n = 1, \dots, N.$$

[26] V. E. and E. Chouzenoux. "Optimized population monte carlo". In: *IEEE Transactions on Signal Processing* 70 (2022), pp. 2489–2501.

O-PMC: Optimized Population Monte Carlo (E. and Chouzenoux, 2022)

Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^N$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^N$ and $\{\mathbf{C}_n\}_{n=1}^N$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$
For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

2. **Weighting:** Weight the NK samples with the DM weights

$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^N q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

[26] V. E. and E. Chouzenoux. "Optimized population monte carlo". In: *IEEE Transactions on Signal Processing* 70 (2022), pp. 2489–2501.

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Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^N$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^N$ and $\{\mathbf{C}_n\}_{n=1}^N$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$
For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

2. **Weighting:** Weight the NK samples with the DM weights

$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

3. **Adaptation of the parameters:**[26]

$$\{\mathbf{C}_{n,j}\}_{n=1}^N \xrightarrow{\text{Hessian of } -log(\widetilde{\pi}(\mathbf{x}))} \{\mathbf{C}_{n,j+1}\}_{n=1}^N$$

$$\{\mathbf{x}_{n,j}^{(k)}, w_{n,j}^{(k)}\}_{n=1,k=1}^{N,K} \xrightarrow{\text{Resampling}} \{\widetilde{\boldsymbol{\mu}}_{n,j}\}_{n=1}^N$$

$$\{\widetilde{\boldsymbol{\mu}}_{n,j}, \mathbf{C}_{n,j}\}_{n=1}^N \xrightarrow{\text{gradient step}} \{\boldsymbol{\mu}_{n,j+1}\}_{n=1}^N$$

Outputs: NKJ weighted samples, $\{\mathbf{x}_{n,j}^{(k)}, w_{n,j}^{(k)}\}_{n=1,k=1,j=1}^{N,K,J}$

[26] V. E. and E. Chouzenoux. "Optimized population monte carlo". In: *IEEE Transactions on Signal Processing* 70 (2022), pp. 2489–2501.

Outline

GRAMIS: Gradient Adaptive Multiple Importance Sampling (E. et al, 2023)

Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^{N}$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^{N}$ and $\{\mathbf{C}_n\}_{n=1}^{N}$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$

[27] V. E., E. Chouzenoux, Ö. D. Akyildiz, and L. Martino. "Gradient-based Adaptive Importance Samplers". In: *Journal of the Franklin Institute (to appear in)* (2023).

GRAMIS: Gradient Adaptive Multiple Importance Sampling (E. et al, 2023)

Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^N$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^N$ and $\{\mathbf{C}_n\}_{n=1}^N$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$

For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

[27] V. E., E. Chouzenoux, Ö. D. Akyildiz, and L. Martino. "Gradient-based Adaptive Importance Samplers". In: *Journal of the Franklin Institute (to appear in)* (2023).

GRAMIS: Gradient Adaptive Multiple Importance Sampling (E. et al, 2023)

Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^N$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^N$ and $\{\mathbf{C}_n\}_{n=1}^N$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$
For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

2. **Weighting:** Weight the NK samples with the DM weights

$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^N q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

[27] V. E., E. Chouzenoux, Ö. D. Akyildiz, and L. Martino. "Gradient-based Adaptive Importance Samplers". In: *Journal of the Franklin Institute (to appear in)* (2023).

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Initialization: Choose J, N, K, $\{q_{n,1}\}_{n=1}^{N}$, $\{\boldsymbol{\mu}_{n,1}\}_{n=1}^{N}$ and $\{\mathbf{C}_n\}_{n=1}^{N}$, e.g., $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{n,1}, \mathbf{C}_n)$

For $j = 1, \ldots, J$**:**

1. **Sampling:** Simulate NK samples as

$$\mathbf{x}_{n,j}^{(k)} \sim q_{n,j}(\mathbf{x}|\boldsymbol{\mu}_{n,j}, \mathbf{C}_n), \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

2. **Weighting:** Weight the NK samples with the DM weights

$$w_{n,j}^{(k)} = \frac{\pi(\mathbf{x}_{n,j}^{(k)})}{\frac{1}{N}\sum_{i=1}^{N} q_{i,j}(\mathbf{x}_{n,j}^{(k)})}, \qquad k = 1, \ldots, K, \qquad n = 1, \ldots, N.$$

3. **Adaptation of the parameters:**[27]

$$\{\mathbf{C}_{n,j}\}_{n=1}^{N} \xrightarrow{\text{Hessian of } -log(\widetilde{\pi}(\mathbf{x}))} \{\mathbf{C}_{n,j+1}\}_{n=1}^{N}$$

$$\{\boldsymbol{\mu}_{n,j}, \mathbf{C}_{n,j}\}_{n=1}^{N} \xrightarrow{\text{gradient step + repulsion among proposals}} \{\boldsymbol{\mu}_{n,j+1}\}_{n=1}^{N}$$

Outputs: NKJ weighted samples, $\{\mathbf{x}_{n,j}^{(k)}, w_{n,j}^{(k)}\}_{n=1,k=1,j=1}^{N,K,J}$

[27] V. E., E. Chouzenoux, Ö. D. Akyildiz, and L. Martino. "Gradient-based Adaptive Importance Samplers". In: *Journal of the Franklin Institute (to appear in)* (2023).

GRAMIS: Gradient Adaptive Multiple Importance Sampling [Elvira23]

- At the j-th iteration of the GRAMIS:
  - Mean adaptation of the n-th proposal:

$$\boldsymbol{\mu}_{n,j} = \boldsymbol{\mu}_{n,j-1} + \mathbf{C}_{n,j-1} \nabla \log\left(\pi(\boldsymbol{\mu}_{n,j-1})\right) + \sum_{i=1, i\neq n}^{N} \mathbf{r}_{n,i}^{(j-1)}, \qquad (1)$$

    with

$$\mathbf{r}_{n,i}^{(j-1)} = G_j \frac{m_n m_i}{\|\mathbf{d}_{n,i}^{(j-1)}\|^{d_x}} \mathbf{d}_{n,i}^{(j-1)}, \qquad (2)$$

    where $\|\cdot\|$ represents the norm operator, $\mathbf{d}_{n,i}^{(j-1)} = \boldsymbol{\mu}_{n,j-1} - \boldsymbol{\mu}_{i,j-1}$, and $m_n, m_i > 0$ are two positive terms that depend on the n-th and i-th proposals respectively.
  - Covariance adaptation of the n-th proposal:

$$\mathbf{C}_{n,j} = \begin{cases} \left(-\nabla^2 \log \pi(\boldsymbol{\mu}_{n,j})\right)^{-1}, & \text{if } \nabla^2 \log \pi(\boldsymbol{\mu}_{n,j}) \succ 0, \\ \mathbf{C}_{n,j-1}, & \text{otherwise.} \end{cases} \qquad (3)$$

Repulsion term in GRAMIS

- Update of location parameter:

$$\boldsymbol{\mu}_{n,j} = \boldsymbol{\mu}_{n,j-1} + \mathbf{C}_{n,j-1}\nabla \log\left(\pi(\boldsymbol{\mu}_{n,j-1})\right) + \sum_{i=1, i\neq n}^{N} G_j \frac{m_n m_i}{\|\mathbf{d}_{n,i}^{(j-1)}\|^{d_x}} \mathbf{d}_{n,i}^{(j-1)}, \ \mathbf{d}_{n,j}^{(j-1)} = \boldsymbol{\mu}_{n,j-1} - \boldsymbol{\mu}_{i,j-1}$$

Repulsion term in GRAMIS

- Modified update of location parameter:

$$\boldsymbol{\mu}_{n,j} = \boldsymbol{\mu}_{n,j-1} + \gamma \nabla \log\left(\pi(\boldsymbol{\mu}_{n,j-1})\right) + \sum_{i=1, i \neq n}^{N} \frac{\gamma}{S_{d_x-1}(1) \|\mathbf{d}_{n,i}^{(j-1)}\|^{d_x}} \mathbf{d}_{n,i}^{(j-1)}, \quad \mathbf{d}_{n,i}^{(j-1)} = \boldsymbol{\mu}_{n,j-1} - \boldsymbol{\mu}_{i,j-1}$$

- Poisson field:

$$-\nabla \varphi^N(\boldsymbol{\mu}_{n,j-1}) = -\int \nabla_u G(\boldsymbol{u}, \boldsymbol{v}) \rho_{n,j-1}^N(\mathrm{d}\boldsymbol{v})$$
$$= \frac{1}{N-1} \sum_{i=1, j \neq n}^{N} \frac{1}{S_{d_x-1}(1)} \frac{\mathbf{d}_{n,i}^{(j-1)}}{\|\mathbf{d}_{n,i}^{(j-1)}\|^{d_x}}$$

  with potential function

$$G(\boldsymbol{u}, \boldsymbol{v}) = \frac{1}{(d_x - 2) S_{d_x-1}(1)} \frac{1}{\|\boldsymbol{u} - \boldsymbol{v}\|^{d_x-2}},$$

  and the empirical measure (of $N-1$ interpreted charges)

$$\rho_{n,j-1}^N(\mathrm{d}\boldsymbol{v}) = \frac{1}{N-1} \sum_{i=1, i \neq n}^{N} \delta_{\boldsymbol{\mu}_{i,j-1}}(\mathrm{d}\boldsymbol{v}),$$

- Summary: the n-th location parameter update balances (a) maximization of π due to $\nabla \log\left(\pi(\boldsymbol{\mu}_{n,j-1})\right)$, and (b) repulsion from all other location parameters due to $-\nabla \varphi_{t-1}^N(\boldsymbol{\mu}_{n,j-1})$

Outline

Mixture of generalized Gaussians

RMSE	AMIS[28]			LR-PMC[29]			O-PMC[30]			GRAMIS[31]		
	η=0.5	η=1	η=1.5	η=0.5	η=1	η=1.5	η=0.5	η=1	η=1.5	η=0.5	η=1	η=1.5
Z	0.969	0.969	0.969	0.012	0.515	0.610	0.009	0.640	0.626	$6.4 \cdot 10^{-4}$	$2.5 \cdot 10^{-6}$	$2.6 \cdot 10^{-3}$
$\mathrm{E}_{\widetilde{\pi}}[\mathbf{X}]$	56.1	56.1	56.1	1.234	50.49	55.2	0.623	56.1	55.5	0.025	$1.5 \cdot 10^{-4}$	0.110
$\mathrm{E}_{\widetilde{\pi}}[\mathbf{X}^2]$	67.95	67.93	68.03	1.12	55.6	65.8	1.029	67.9	66.6	1.296	0.002	0.188
$\chi^2\left(\widetilde{\pi}, \psi^{(T)}\right)$	980.1	980.1	980.1	30.6	556.7	616.8	7.84	639.9	630.3	0.778	0.005	4.34

Table: **Mixture of 5 generalized Gaussians.** RMSE of the IS estimators. In the case of GRAMIS, $G_1 = 1$ with exponential decay. The MSE results are obtained over 100 independent runs, with estimators using the weighted samples on the half last iterations.

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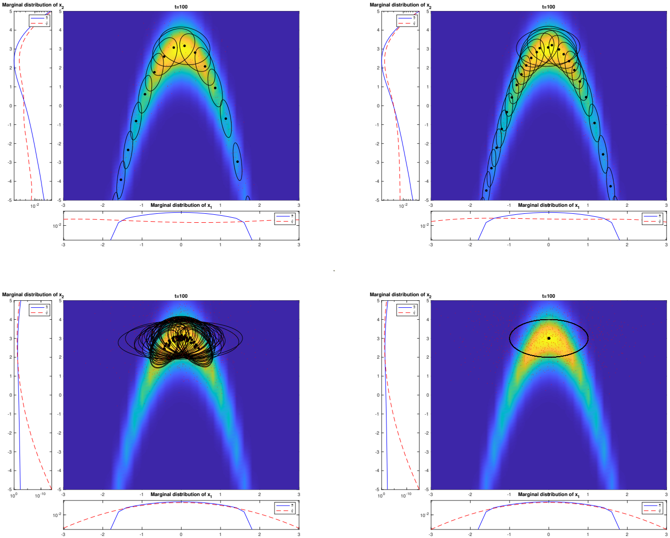
[29] V. E., L. Martino, D. Luengo, and M. F. Bugallo. "Improving population Monte Carlo: Alternative weighting and resampling schemes". In: *Signal Processing* 131 (2017), pp. 77–91.

[30] V. E. and E. Chouzenoux. "Optimized population monte carlo". In: *IEEE Transactions on Signal Processing* 70 (2022), pp. 2489–2501.

[31] V. E., E. Chouzenoux, Ö. D. Akyildiz, and L. Martino. "Gradient-based Adaptive Importance Samplers". In: *Journal of the Franklin Institute (to appear in)* (2023).

GRAMIS in banana-shaped distribution (repulsion study)



[32] V. E., E. Chouzenoux, Ö. D. Akyildiz, and L. Martino. "Gradient-based Adaptive Importance Samplers". In: *Journal of the Franklin Institute (to appear in)* (2023).

Outline

Conclusion

- IS is a powerful methodology but requires the adaptation of the proposal(s).
- AIS methods have grown greatly in the last decade with new daptive mechanisms:
  - standard MCMC algorithms
  - HMC
  - Langevin dynamics
  - variational algorithms
  - interpretations from physical systems
  - ...
- We should probably drop the dichotomy between
  - optimization and sampling techniques
  - MCMC and IS

Thank you for your attention!

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O-PMC. V. E., E. Chouzenoux, "Optimized Population Monte Carlo", IEEE Transactions on Signal Processing, Vol. 70, pp. 2489 - 2501, 2022.

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