Nested expectations with kernel quadrature

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$$I := \int_{\Theta} f\left(\int_{\mathcal{X}} g(x,\theta)p_{\theta}(x)dx\right)q(\theta)d\theta\,.$$

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- I will be using only one level of nesting for simplicity, but we may sometimes care about more…

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$$I := \int_{\Theta} f\left(\int_{\mathcal{X}} g(x,\theta)p_\theta(x)dx\right)q(\theta)d\theta$$

→ Batch active learning/Bayesian optimisation (inner: acquisition function for 1st point, outer: acquisition function for 2nd point given 1st point)

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$$I := \int_{\Theta} f\left(\int_{\mathcal{X}} g(x,\theta)p_\theta(x)dx\right)q(\theta)d\theta$$

→ Statistical divergences for conditional distributions (inner: standard statistical divergence, outer: average over conditioning variable)

Examples in Stats/ML/UQ

$$I := \int_{\Theta} f\left(\int_{\mathcal{X}} g(x, \theta) p_{\theta}(x) dx\right) q(\theta) d\theta$$

→ Bayesian distributionally robust optimisation (inner: expected risk against model, outer: expectation over posterior)

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→ Bayesian experimental design (inner: information gain - expectation over posterior, outer: expected information gain - expectation over marginal predictive distribution)

Examples in other fields

$$I := \int_{\Theta} f\left(\int_{\mathcal{X}} g(x,\theta)p_{\theta}(x)dx\right)q(\theta)d\theta$$

→ Option pricing (inner: expected loss given shock , outer: expectation over distribution of potential shocks)

Examples in other fields

$$I := \int_{\Theta} f\left(\int_{\mathcal{X}} g(x,\theta)p_{\theta}(x)dx\right)q(\theta)d\theta$$

→ Health economics - Expected value of partial perfect information (inner: expected patient outcome given variable of interest, outer: expectation over prior beliefs about variable of interest)

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→ ......

Some desiderata

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- We define the **cost** of a method as the # function evaluations/samples needed for:

$$\begin{cases} \text{Absolute error} = |I - \hat{I}| \leq \Delta \\ \text{RMSE } = \sqrt{\mathbb{E}[(I-\hat{I})^2]} \leq \Delta \end{cases}$$

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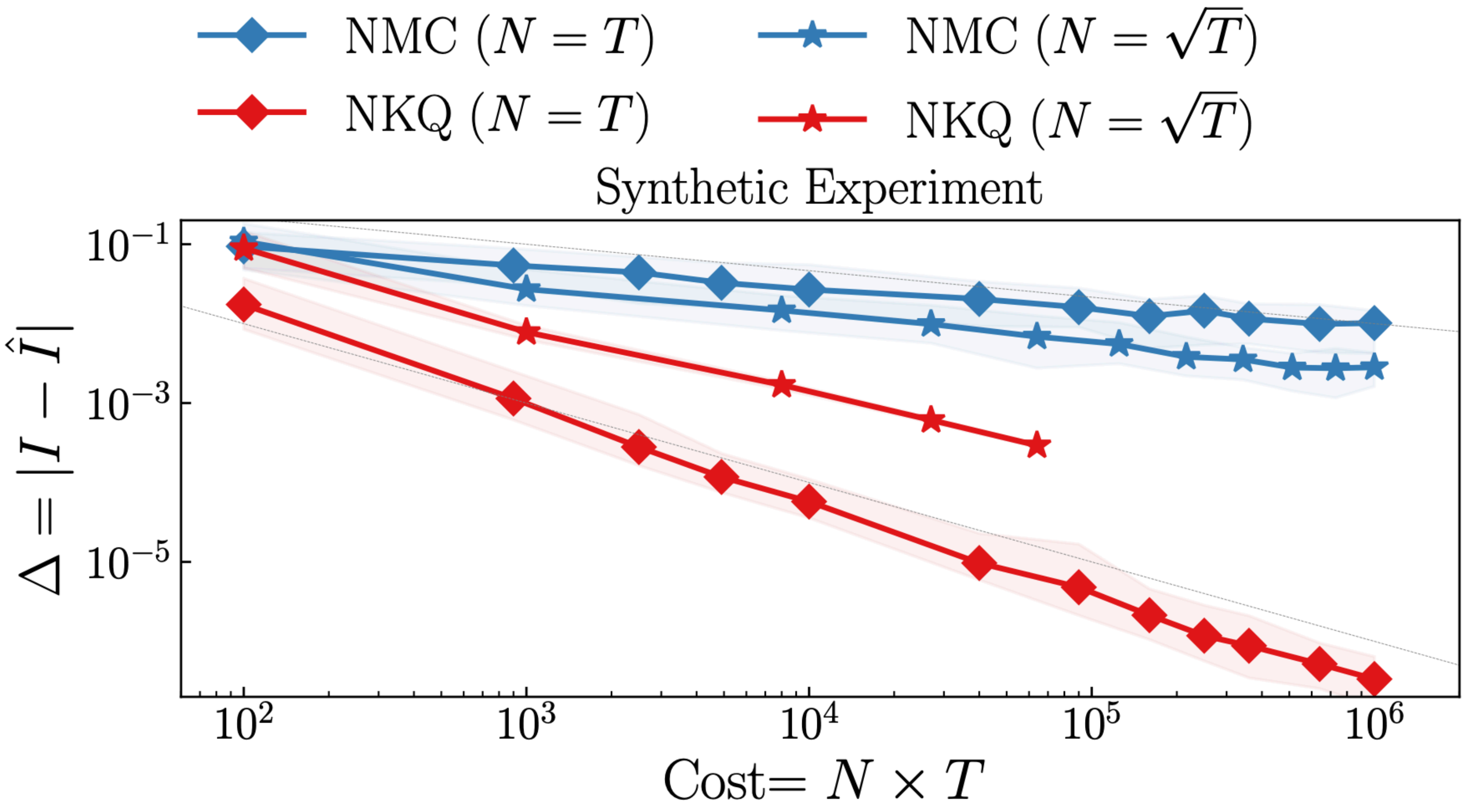
→ This is very important as most existing estimators tend to be **very** expensive.

What to expect….

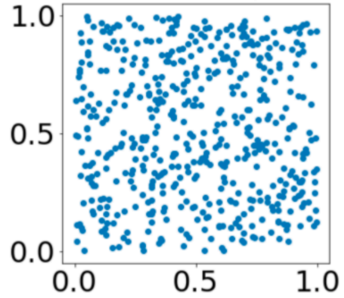


$$g(x,\theta) = x^{\frac{5}{2}} + \theta^{\frac{5}{2}}$$

$$f(z) = z^2$$

$$\mathbb{Q} = \mathbb{P}_\theta = U[0,1]$$

Nested Monte Carlo



The most obvious estimator:

IID samples:

$$\theta_{1:T} = (\theta_1, \ldots, \theta_T)^\top \sim \mathbb{Q}$$

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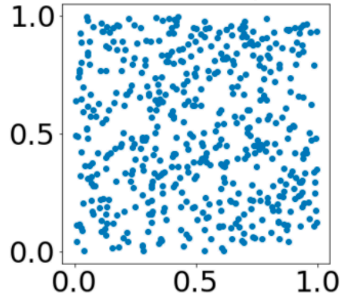

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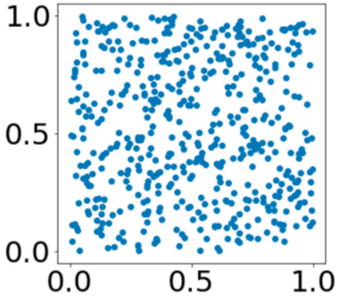

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inner Monte Carlo outer Monte Carlo

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- **Note:** This is biased since we never get to evaluate:

$$f\left(\int_{\mathcal{X}} g(x,\theta)p_\theta(x)dx\right)$$

Convergence of Nested Monte Carlo (ctd)

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Smaller than 4, but still quite large

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Nested quasi Monte Carlo

QMC points:

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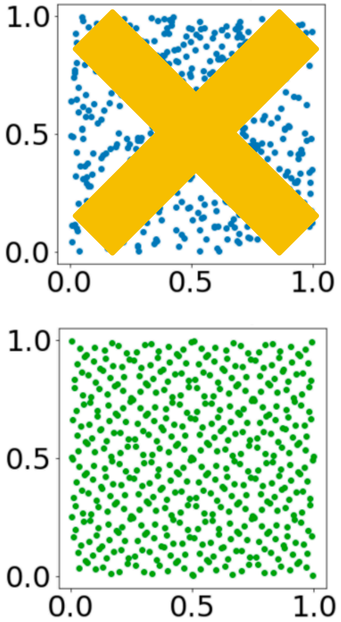

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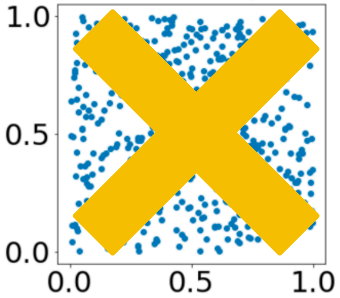

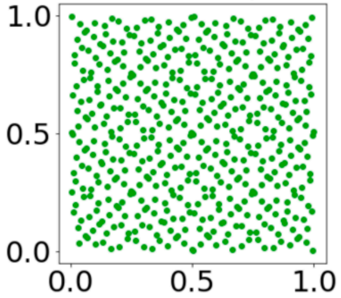

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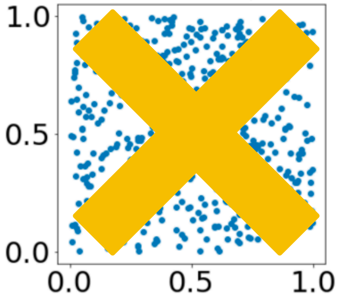

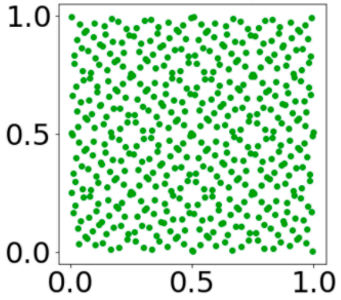

➜ Limited to cases where $\mathscr{X} = [0,1]^{d_{\mathscr{X}}}$, $\Theta = [0,1]^{d_\theta}$ and uniform measures.

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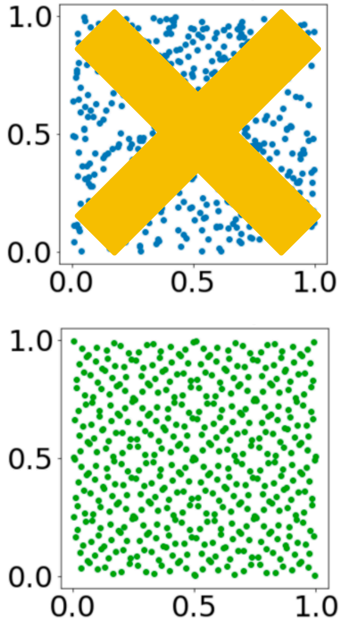

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- Limited to cases where $\mathscr{X} = [0,1]^{d_\mathscr{X}}$, $\Theta = [0,1]^{d_\theta}$ and uniform measures.
- Can get $\text{Cost}\left(\hat{I}_{\text{NQMC}}\right) = O\left(\Delta^{-2.5}\right)$ but requires **very strong** assumptions on f (second and third derivatives are monotone).

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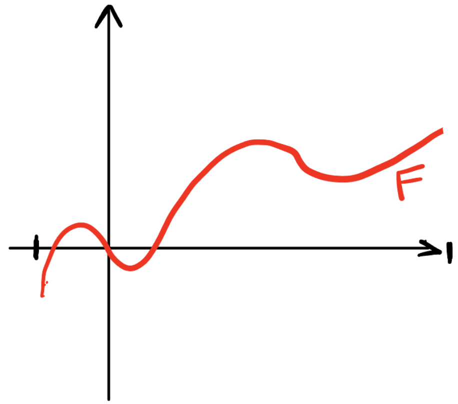
Multi-level Monte Carlo



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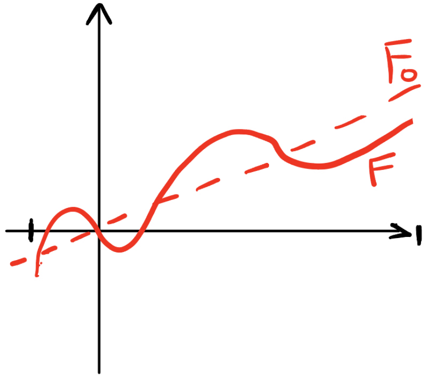

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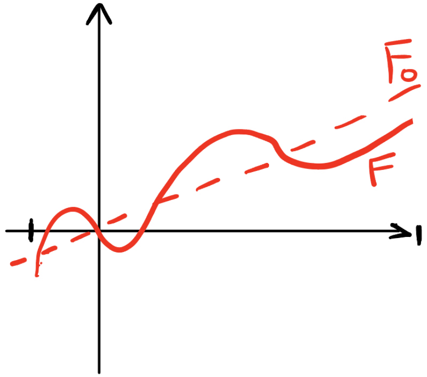

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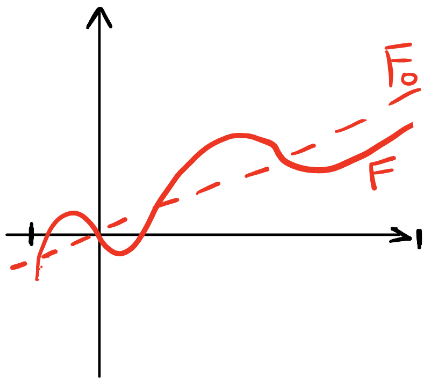

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Giles, M. B. (2015). Multilevel Monte Carlo methods. *Acta Numerica*, *24*, 259–328.

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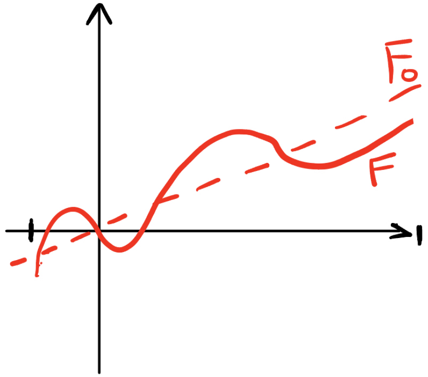

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High variance

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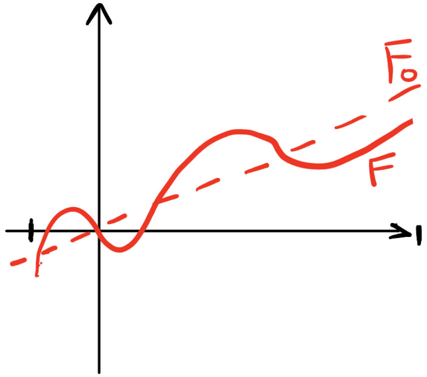

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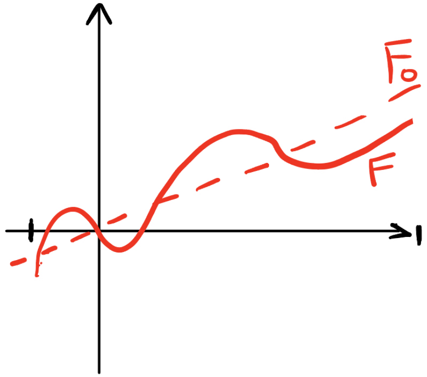

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(Very) small variance

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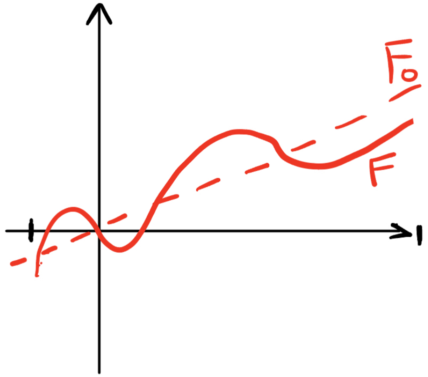

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$$I := \int_\Theta F(\theta)q(\theta)d\theta \;= \int_\Theta F_0(\theta)q(\theta)d\theta + \sum_{l=1}^{L}\int_\Theta (F_l(\theta) - F_{l-1}(\theta))q(\theta)d\theta$$

$$\approx \frac{1}{\boxed{T_0}}\sum_{t=1}^{T_0}\boxed{F_0(\theta_t^0)} + \sum_{l=1}^{L}\frac{1}{\boxed{T_l}}\sum_{t=1}^{T_l}\boxed{(F_l(\theta_t^l) - F_{l-1}(\theta_t^l))}$$

(Very) small variance

High variance

Small since expensive

Large since cheap

Giles, M. B. (2015). Multilevel Monte Carlo methods. *Acta Numerica*, *24*, 259–328.

MLMC for nested expectations

IID points:
$$\theta_{1:T} = (\theta_1, \ldots, \theta_T)^\top$$
$$x^{(t)}_{1:N} = (x^{(t)}_1, \ldots, x^{(t)}_N)^\top \sim \mathbb{P}_{\theta_t}, \quad t \in \{1,\ldots,T\}$$

Define:
$$F(\theta) := f\left(\int g(x,\theta) p_\theta(x) dx\right) \quad F_l(\theta) := f\left(\frac{1}{N_l}\sum_{n=1}^{N_l} g(x_n, \theta)\right)$$

Giles, M. B. (2015). Multilevel Monte Carlo methods. *Acta Numerica*, *24*, 259–328. (Chapter 9)

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→ Can get much lower cost: $\text{Cost}\left(\hat{I}_{\text{MLMC}}\right) = O\left(\Delta^{-2}\right)$

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Much better than NMC/NQMC!

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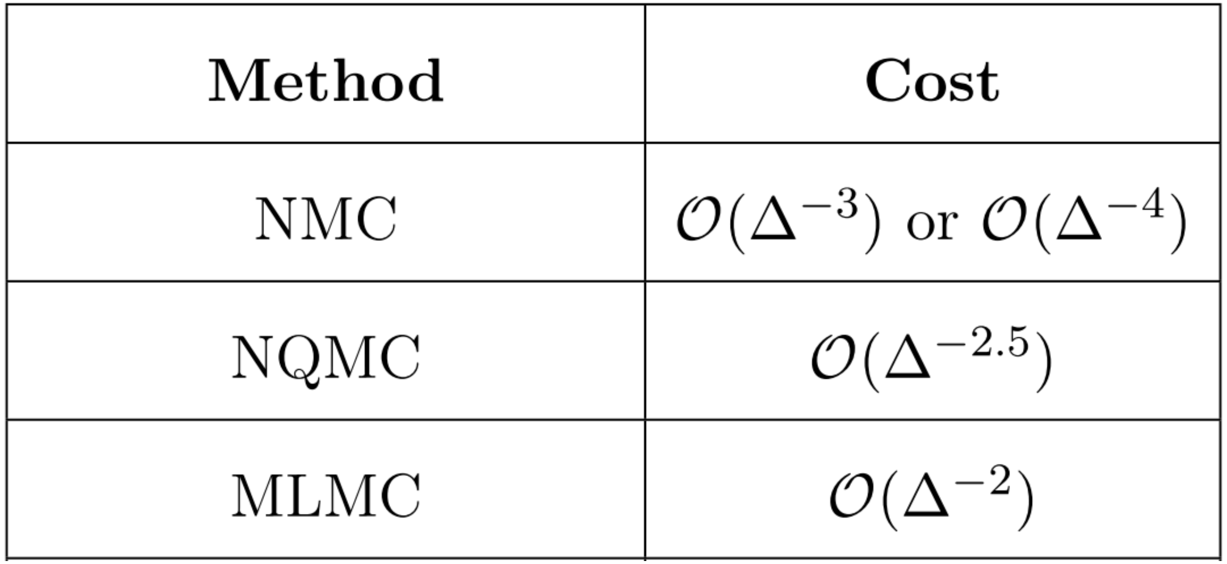
Giles, M. B. (2015). Multilevel Monte Carlo methods. *Acta Numerica*, *24*, 259–328. (Chapter 9)

A comparison of convergence rates



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NMC	$\mathcal{O}(\Delta^{-3})$ or $\mathcal{O}(\Delta^{-4})$
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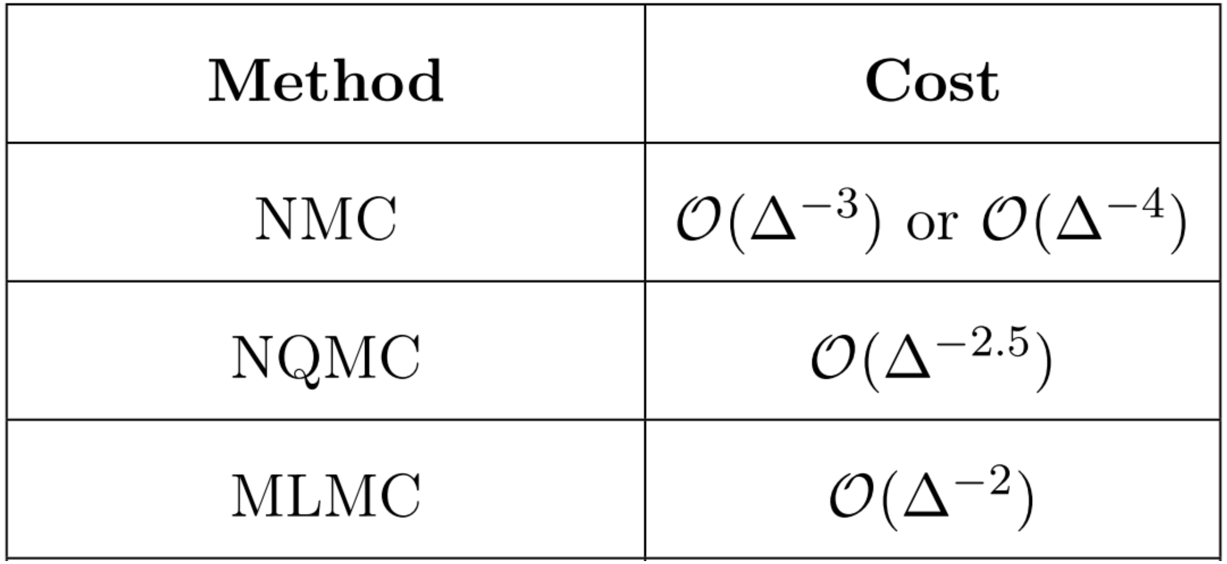

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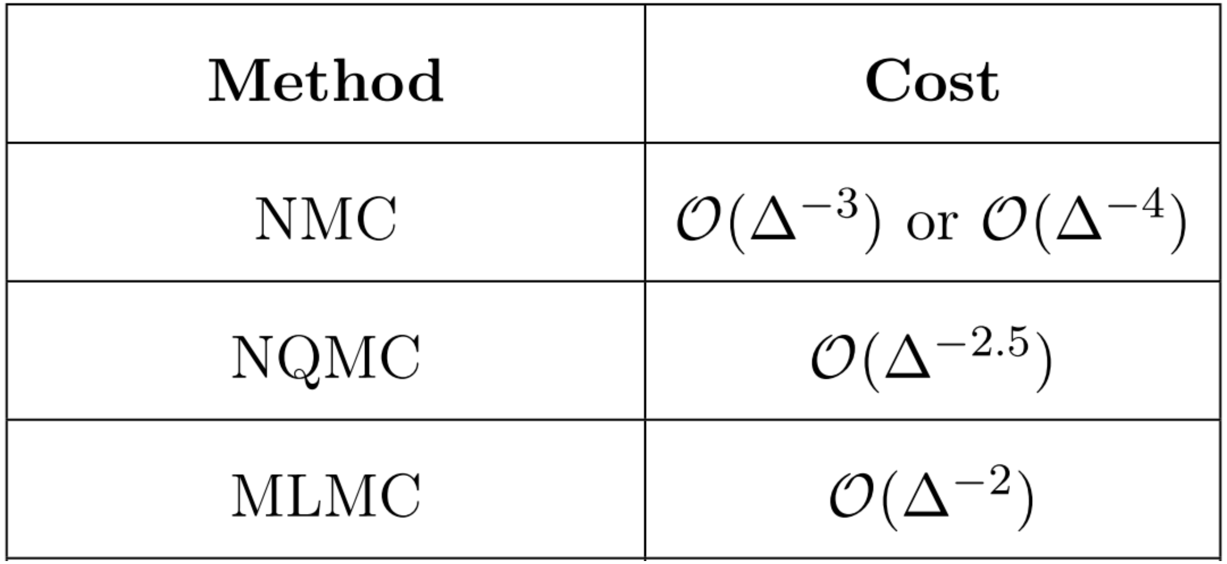

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($\tilde{O}$ means I am hiding log terms)

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Smaller than 2 for sufficiently smooth integrands!

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$O(10^4)$ evaluations

$O(10^2)$ or $O(10^3)$ evaluations?

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Quadrature rules

Quantity of interest:

$$I = \int_{\mathcal{X}} h(x)\pi(x)dx$$

Data:

$$x_{1:N} := \left[x_1, \cdots, x_N\right]^\top \in \mathcal{X}^N,$$

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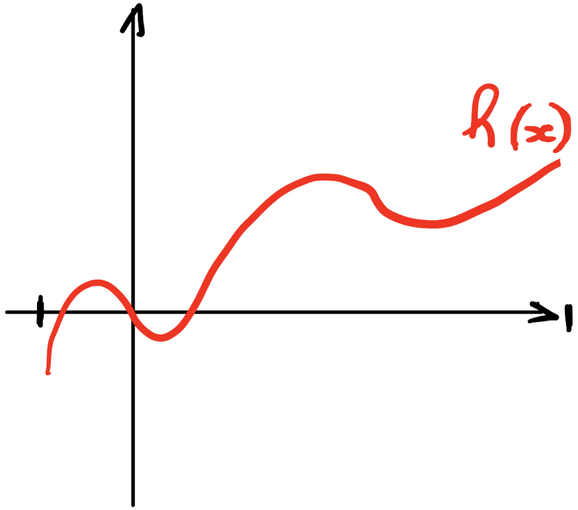

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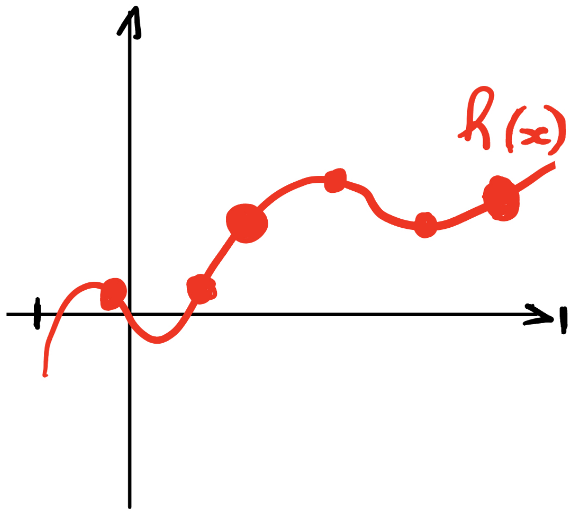

Quadrature rule:
$$\hat{I} = \sum_{i=1}^{N} w_i h(x_i)$$

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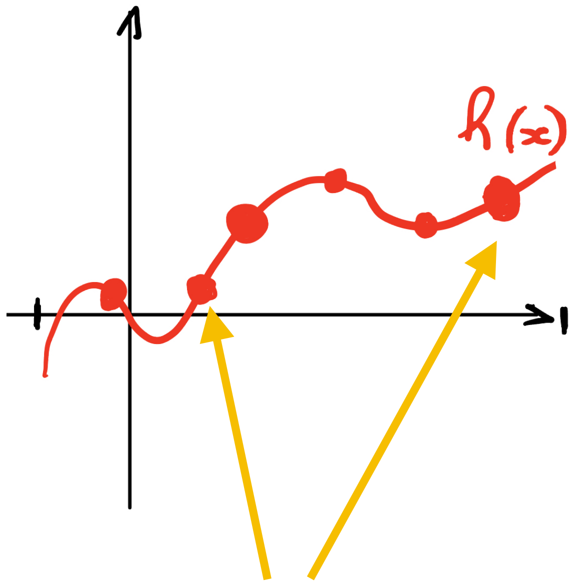
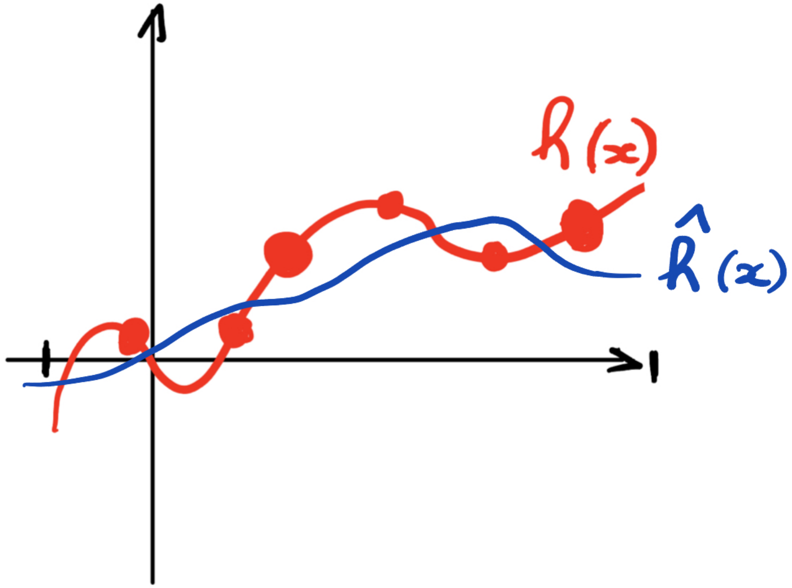


Weight w_i depends on x_i!

Kernel Quadrature (KQ)

- Compute a kernel ridge regression estimator of h using some reproducing kernel k:

$$\hat{h}(x) := k(x, x_{1:N})(k(x_{1:N}, x_{1:N}) + N\lambda I_N)^{-1} h(x_{1:N})$$



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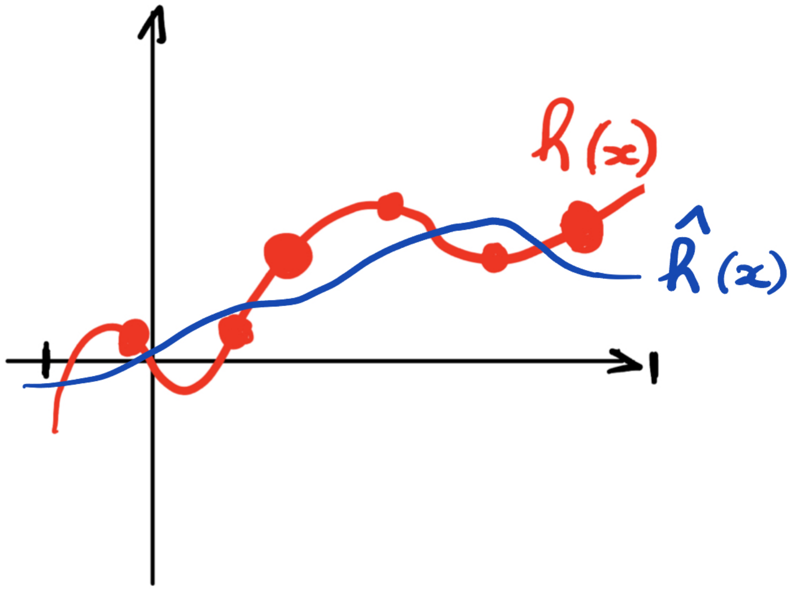
Gram matrix



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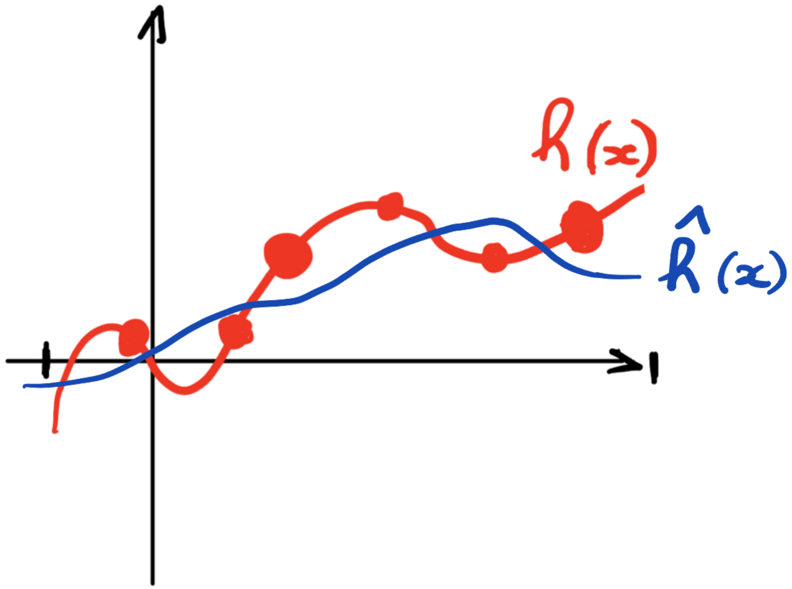

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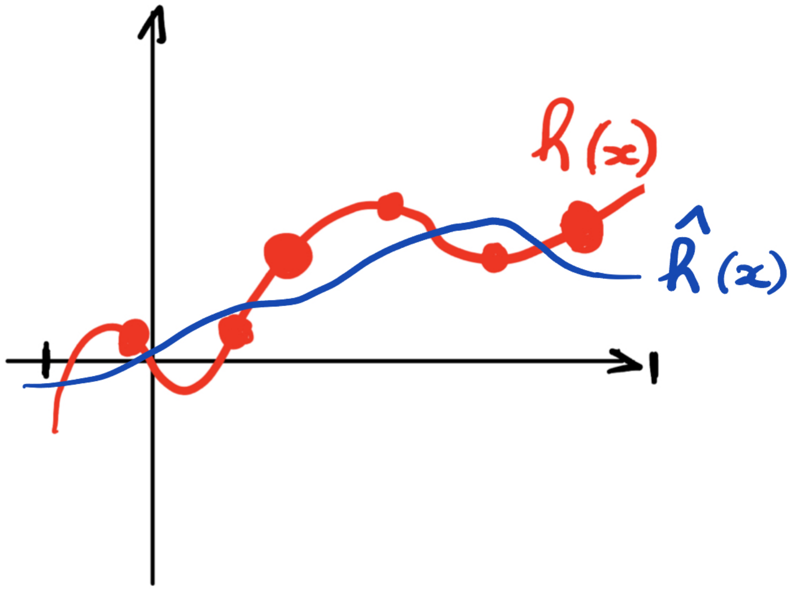

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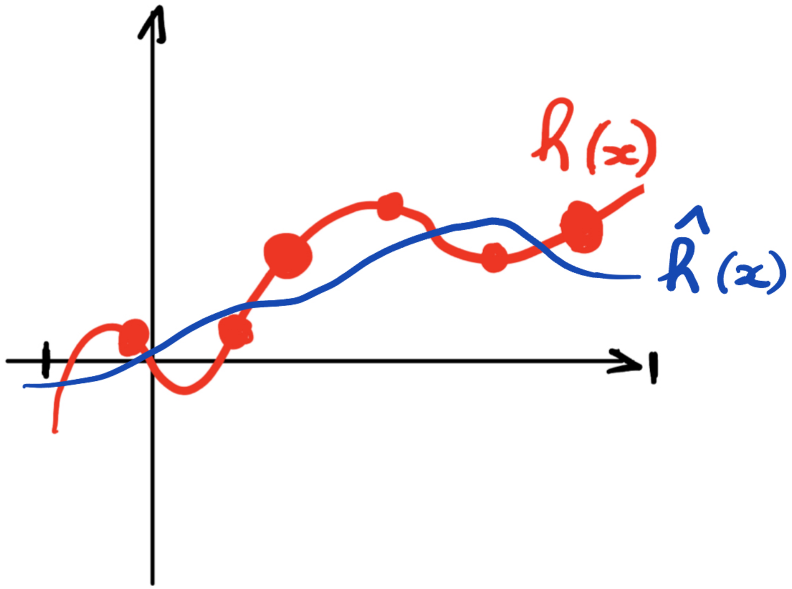

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Gram matrix Regulariser Identity matrix

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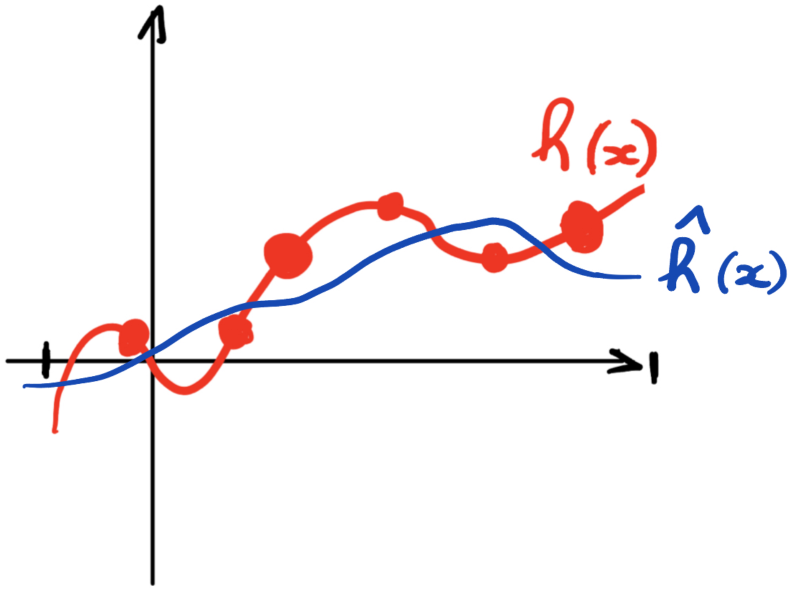

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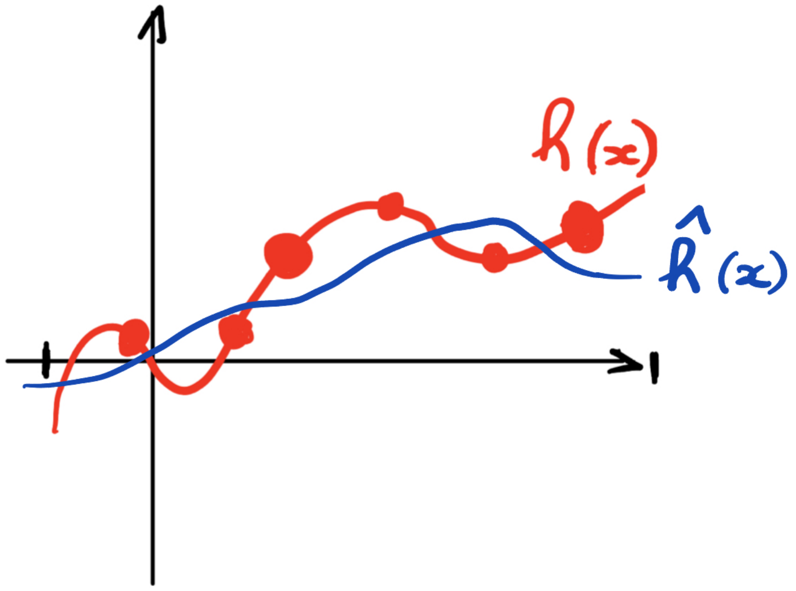

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Kernel mean embedding!

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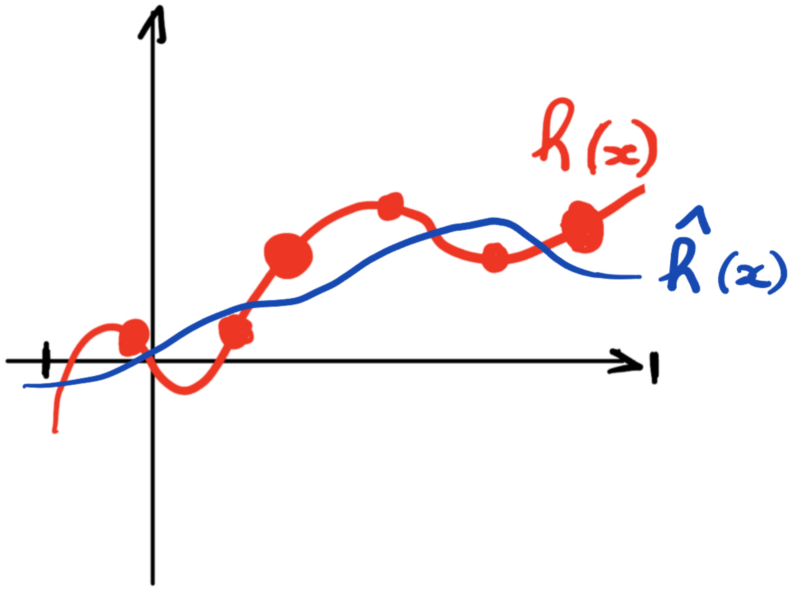

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Kernel mean embedding!

- Closely relates to Bayesian quadrature (same procedure but with GP regression).

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Closed-form embeddings

We need closed-form kernel mean embeddings; this is not always straightforward!

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Anastasiou, A., et al. (2023). Stein's method meets computational statistics: A review of some recent developments. Statistical Science, 38(1), 120–139.

Briol, F-X., Gessner, A., Karvonen, T., Mahsereci, M (2025). A dictionary of closed-form kernel mean embeddings. (to appear; next week?)

Advantages/Disadvantages of KQ

Disadvantages:

- Computational cost is $O(N^3)$ in the worst-case due to matrix inversion.
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Advantages:

- Typically converges much faster than alternative estimators when integrand is smooth and not too high-dimensional!

Nested Kernel Quadrature

Stage I: Compute KQ estimators (with $k_{\mathcal{X}}$) for inner expectations; i.e. for integrals of $g(\,\cdot\,, \theta_1), \ldots, g(\,\cdot\,, \theta_T)$.

Denote these $\hat{J}_{\mathsf{KQ}}(\theta_1), \ldots, \hat{J}_{\mathsf{KQ}}(\theta_T)$.

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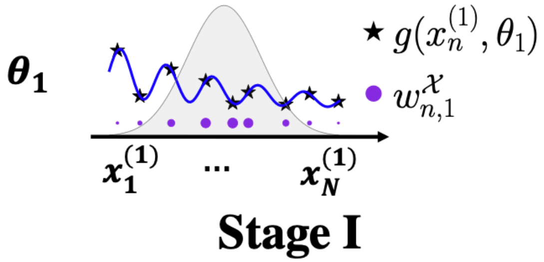

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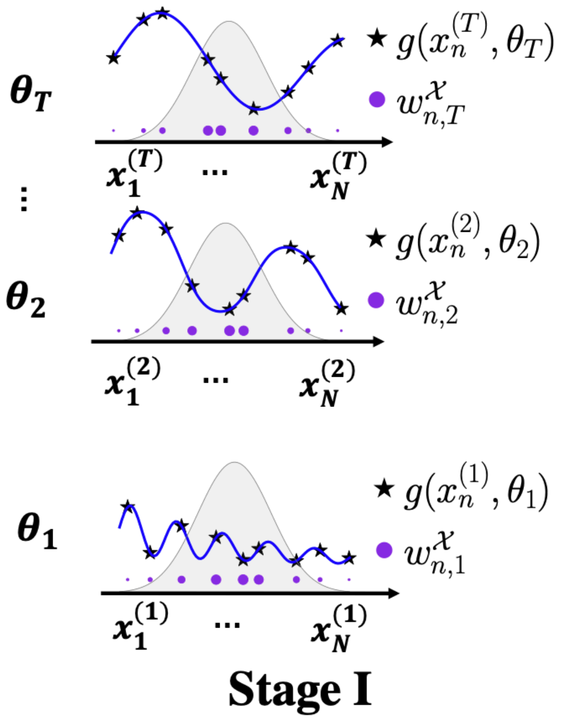

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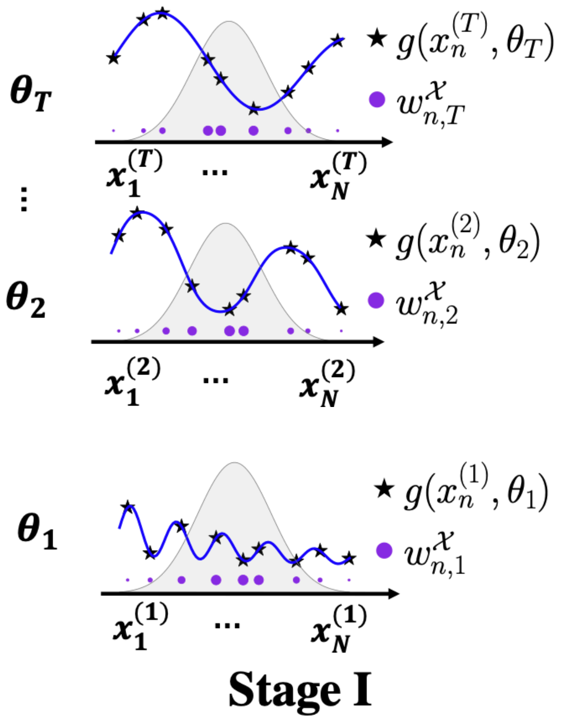
Stage II: Compute a KQ estimator (with k_Θ) for outer expectation; i.e. integral of

$$F(\theta) = f\left(\int_{\mathcal{X}} g(x, \theta) p_\theta(x) dx \right)$$

using noisy data from stage I:

$$\hat{F}_{\text{KQ}}(\theta_t) = f\left(\hat{J}_{KQ}(\theta_t)\right) \approx F(\theta_t)$$



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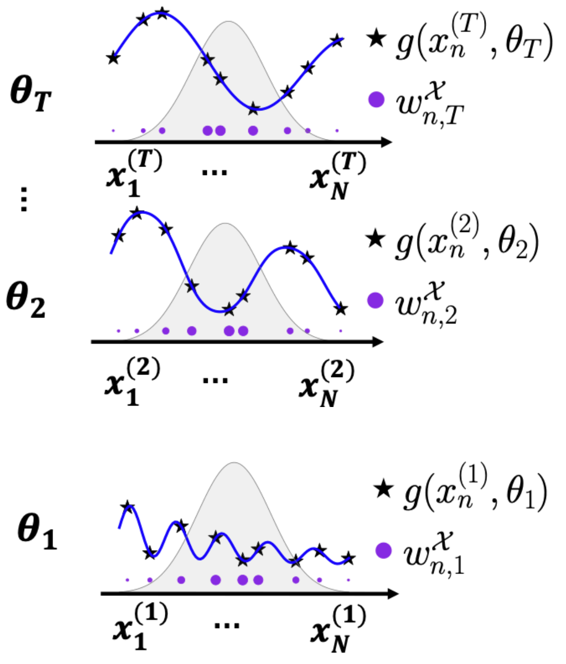

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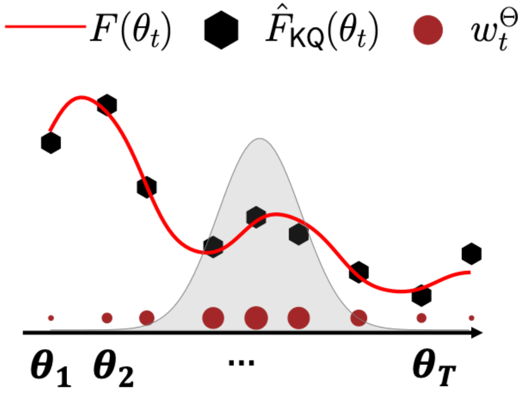


Stage II

Nested Kernel Quadrature

Stage I: Compute KQ estimators (with $k_{\mathcal{X}}$) for inner expectations; i.e. for integrals of $g(\cdot, \theta_1), \ldots, g(\cdot, \theta_T)$.

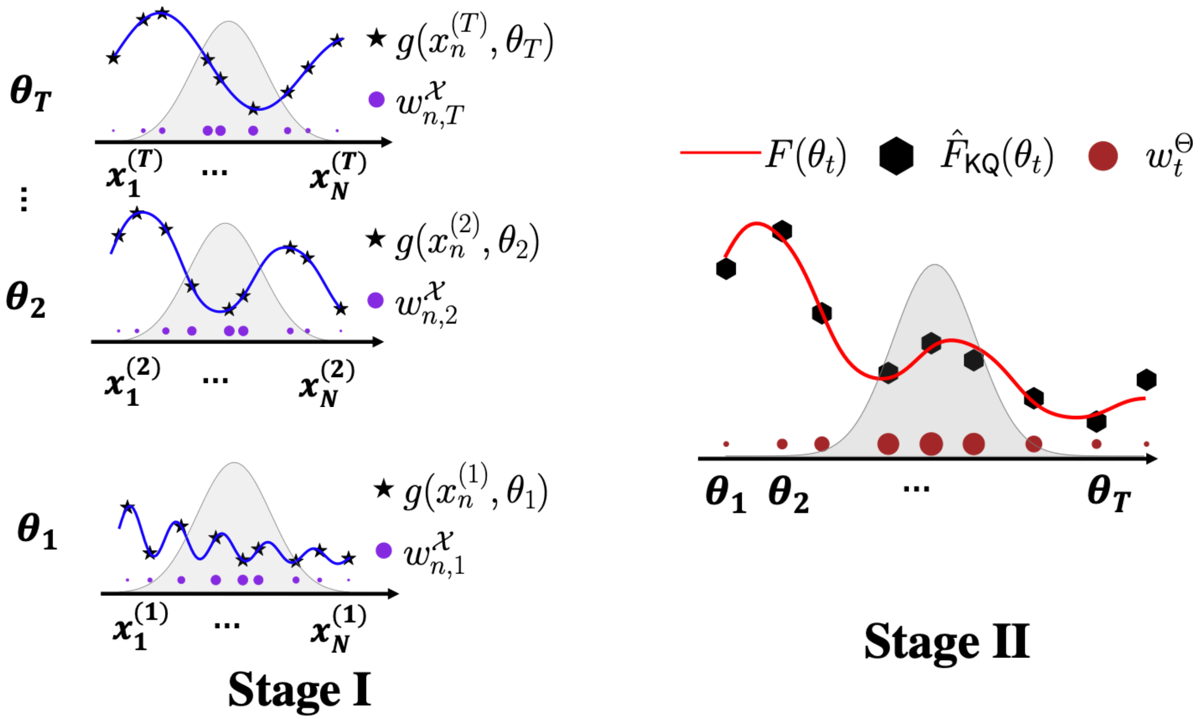
Denote these $\hat{J}_{\mathrm{KQ}}(\theta_1), \ldots, \hat{J}_{\mathrm{KQ}}(\theta_T)$.

Stage II: Compute a KQ estimator (with k_Θ) for outer expectation; i.e. integral of

$$F(\theta) = f\left(\int_{\mathcal{X}} g(x, \theta) p_\theta(x) dx\right)$$

using noisy data from stage I:

$$\hat{F}_{\mathrm{KQ}}(\theta_t) = f\big(\hat{J}_{KQ}(\theta_t)\big) \approx F(\theta_t)$$



$$\hat{I}_{\mathrm{NKQ}} = \sum_{t=1}^{T} w_t^\Theta f\left(\sum_{i=1}^{N} w_{n,t}^{\mathcal{X}} g(x_n^{(t)}, \theta_t)\right)$$

Convergence guarantees for NKQ

- **Theorem (informal):** Let $\mathscr{X} = [0,1]^{d_\mathscr{X}}$ and $\Theta = [0,1]^{d_\Theta}$. Under regularity assumptions including

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  - $x \mapsto D_\theta^\beta g(x,\theta)$ has smoothness $s_\mathcal{X}$ for all $\beta \in \mathbb{N}_0^{d_\Theta}$ with $|\beta| \leq s_\Theta$.

Convergence guarantees for NKQ

Then, taking $\lambda_{\mathcal{X}} = \tilde{O}(N^{-\frac{2s_{\mathcal{X}}}{d_{\mathcal{X}}}})$ and $\lambda_{\Theta} = \tilde{O}(T^{-\frac{2s_{\Theta}}{d_{\Theta}}})$, we get that for N, T large enough the following holds with high prob:

$$\Delta = \left| \hat{I}_{\text{NKQ}} - I \right| = \tilde{O}\left(N^{-\frac{s_{\mathcal{X}}}{d_{\mathcal{X}}}} + T^{-\frac{s_{\Theta}}{d_{\Theta}}} \right)$$

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Fast! Much better than MC!

Cost of NKQ

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- This **fast (interpolation-type) rate is surprising** given we are using **noisy function values** for approximating the outer expectation, so we should expect a regression rate!

Fischer, S., & Steinwart, I. (2020). Sobolev norm learning rates for regularized least-squares algorithm. *Journal of Machine Learning Research*, *21*(205), 1–38.

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- Recall that $s_{\mathcal{X}} \geq d_{\mathcal{X}}/2$ and $s_\Theta \geq d_\Theta/2$, so we get at worse the NMC rate: $\tilde{O}\left(\Delta^{-4}\right)$

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→ When $s_{\mathcal{X}}$ and s_{Θ} are large enough, we can beat NQMC and MLMC!

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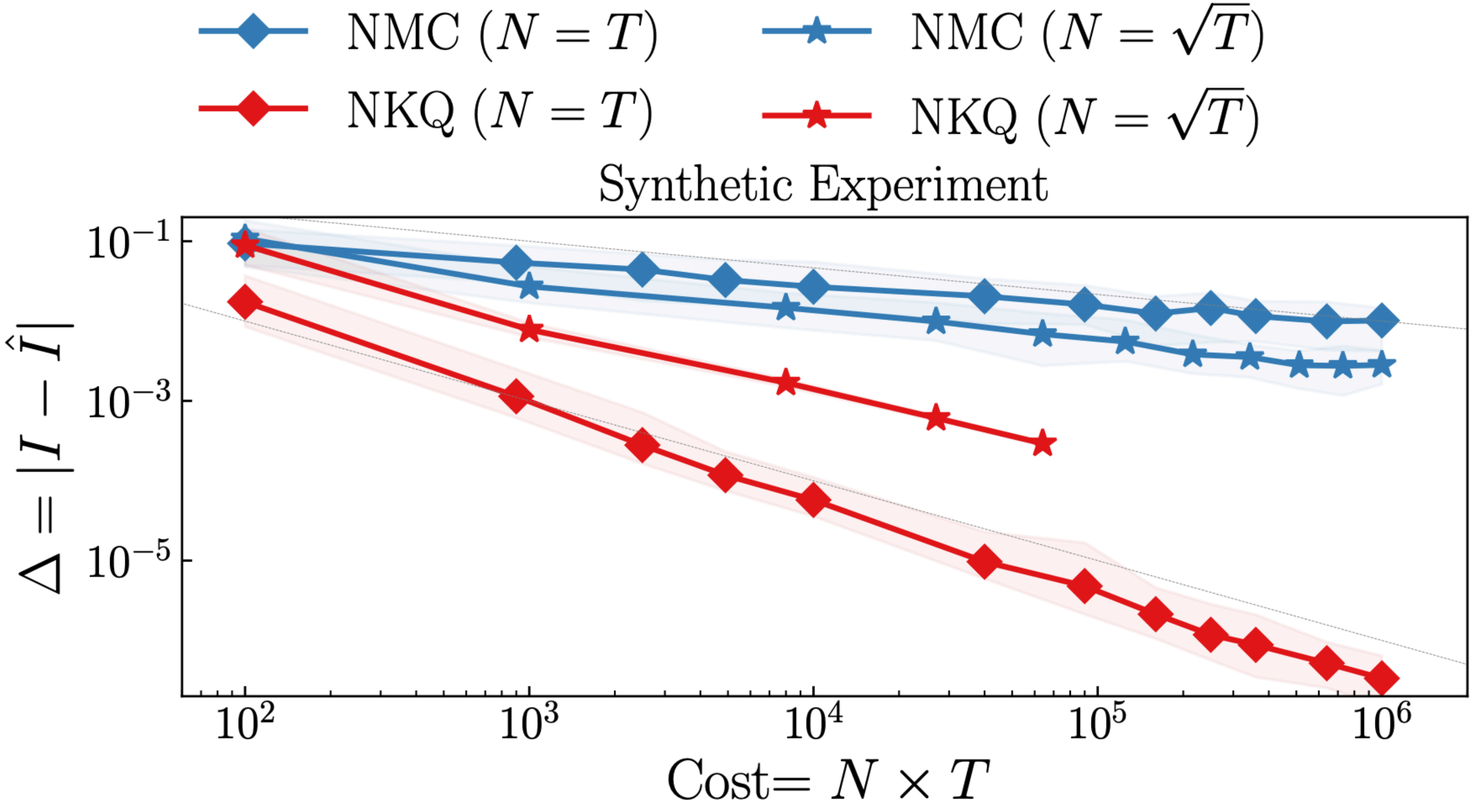
Back to the synthetic experiment

$$g(x, \theta) = x^{\frac{5}{2}} + \theta^{\frac{5}{2}}$$

$$f(z) = z^2$$

$$\mathbb{Q} = \mathbb{P}_\theta = U[0,1]$$



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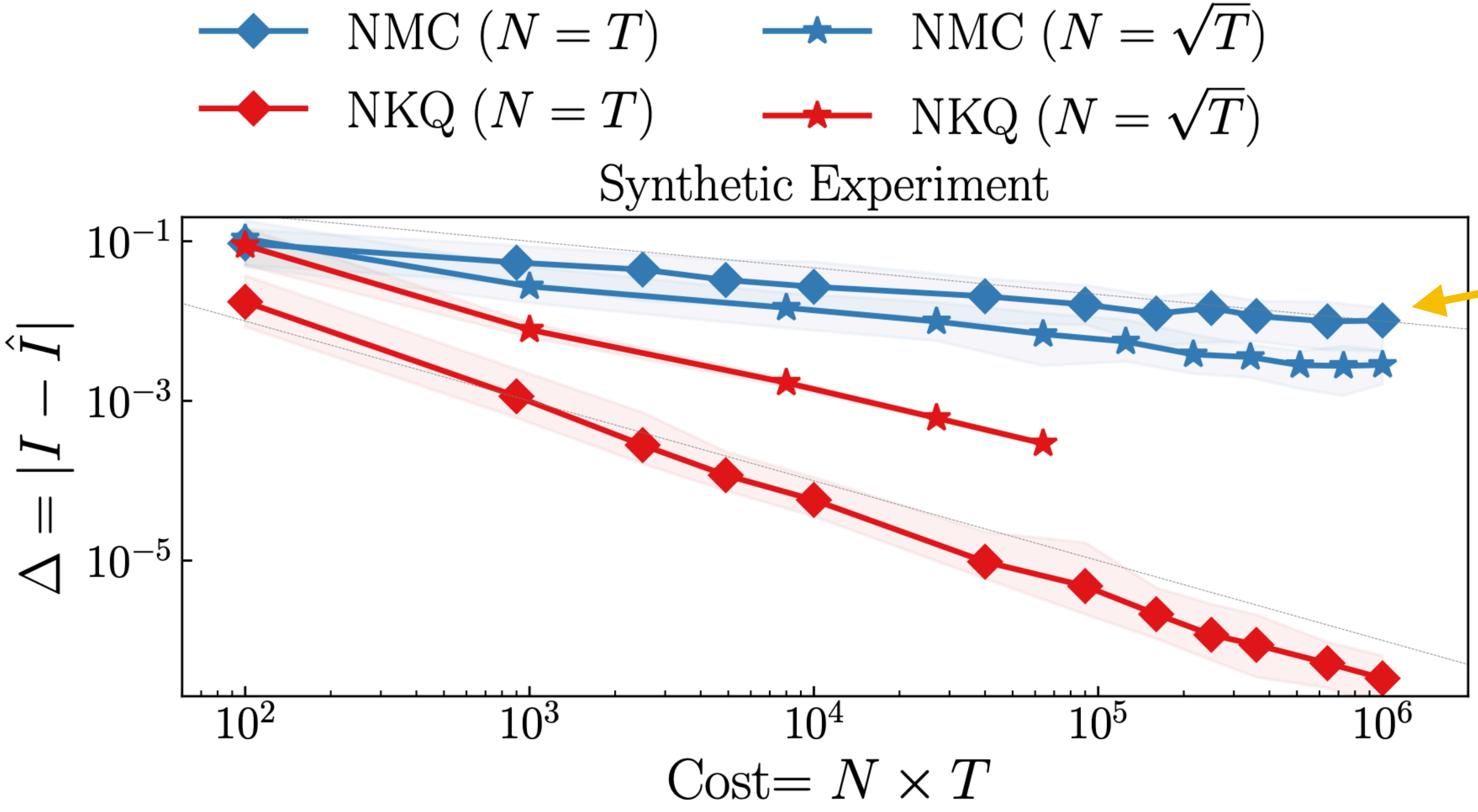

As predicted by NMC theory, $N = T$ gives the slower rate: $O(\Delta^{-4})$

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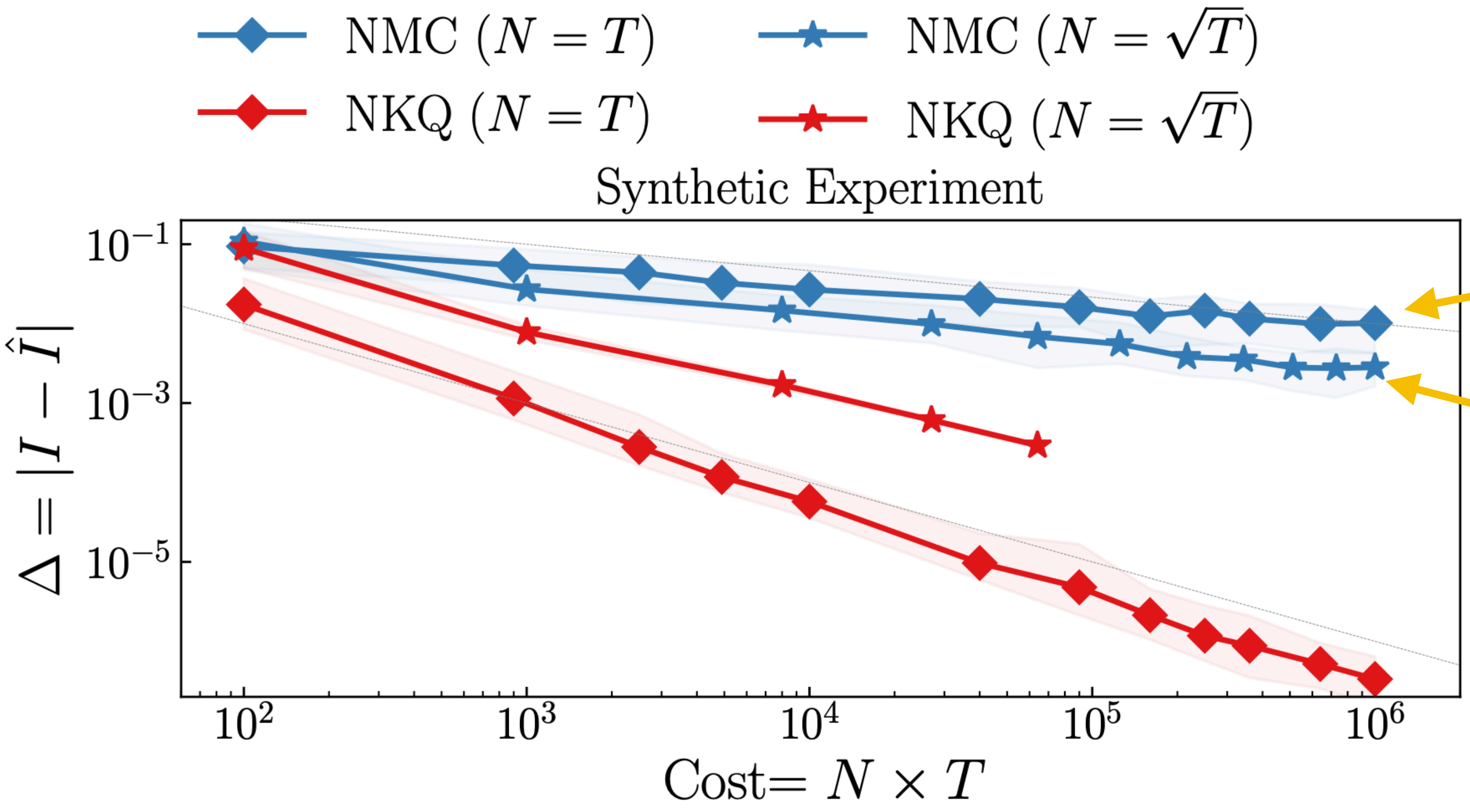

As predicted by NMC theory, $N = T$ gives the slower rate: $O(\Delta^{-4})$

Taking $N = \sqrt{T}$ gives the faster rate: $O(\Delta^{-3})$ since integrand nice.

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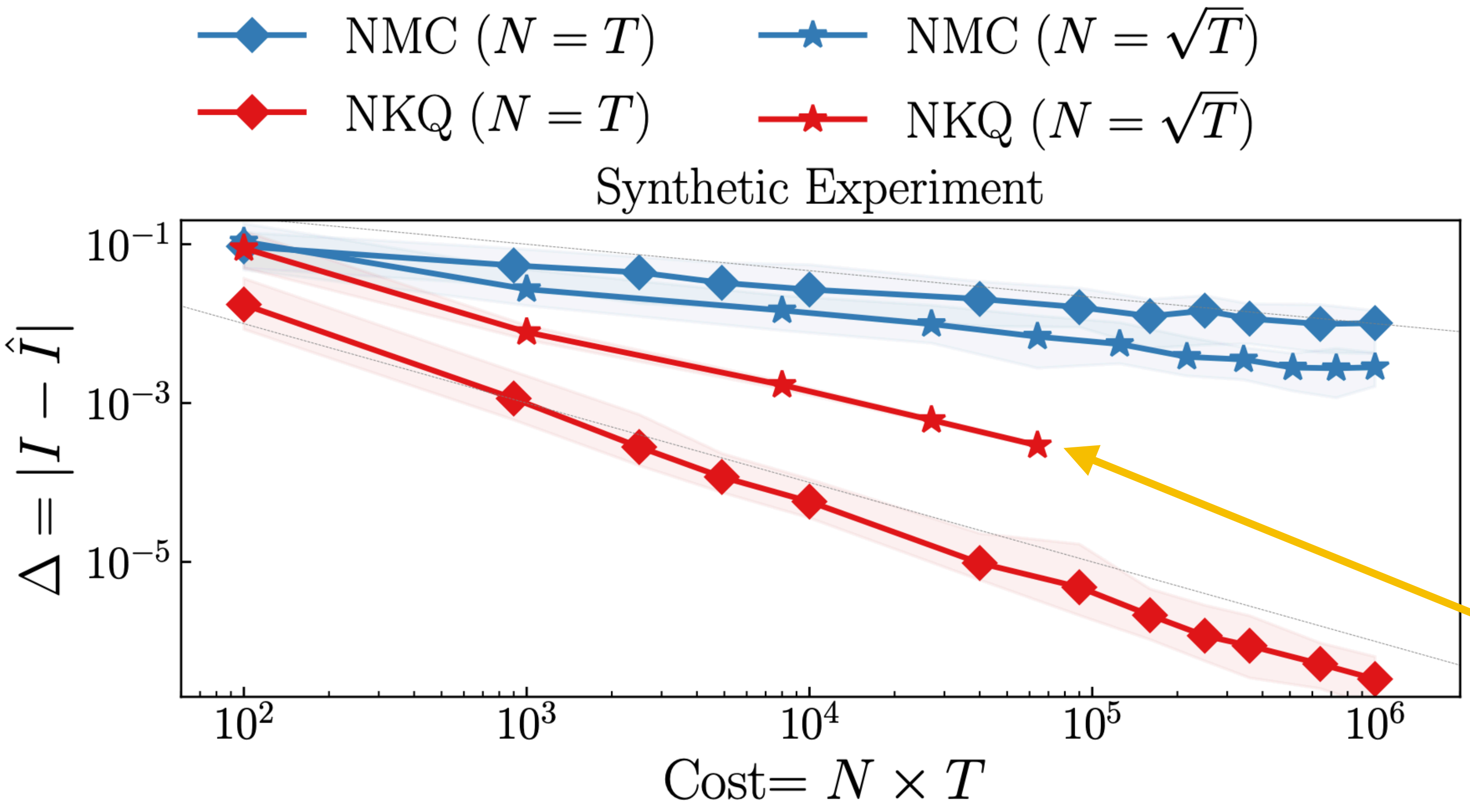

For NKQ, $N = \sqrt{T}$ is sub-optimal.

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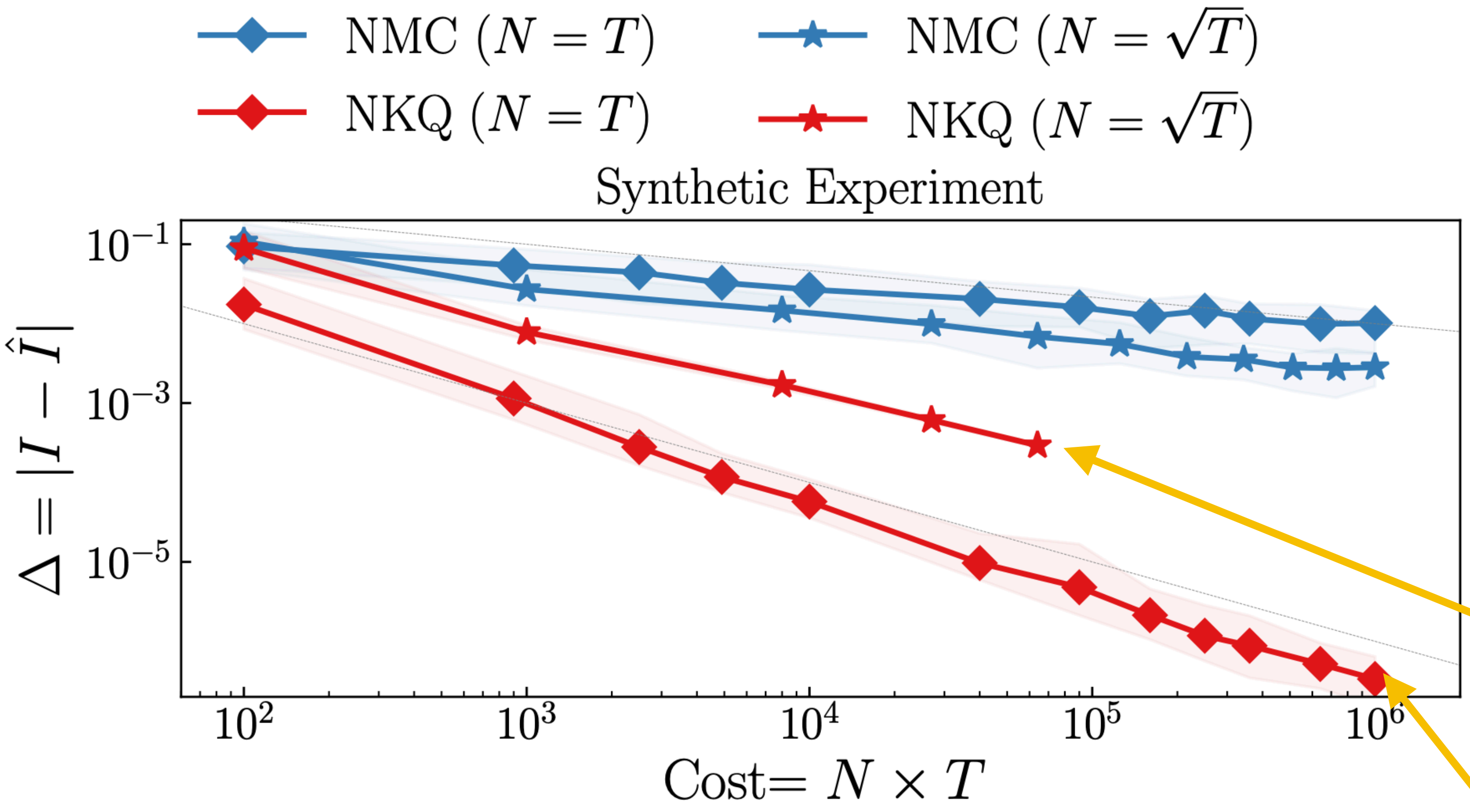

For NKQ, $N = \sqrt{T}$ is sub-optimal.

As predicted by our theorem, $N = T$ gives a fast rate!

We suffer in high dimensions…

$$g(x,\theta) = \|x\|_2^{\frac{5}{2}} + \|\theta\|_2^{\frac{5}{2}}$$

$$f(z) = z^2$$

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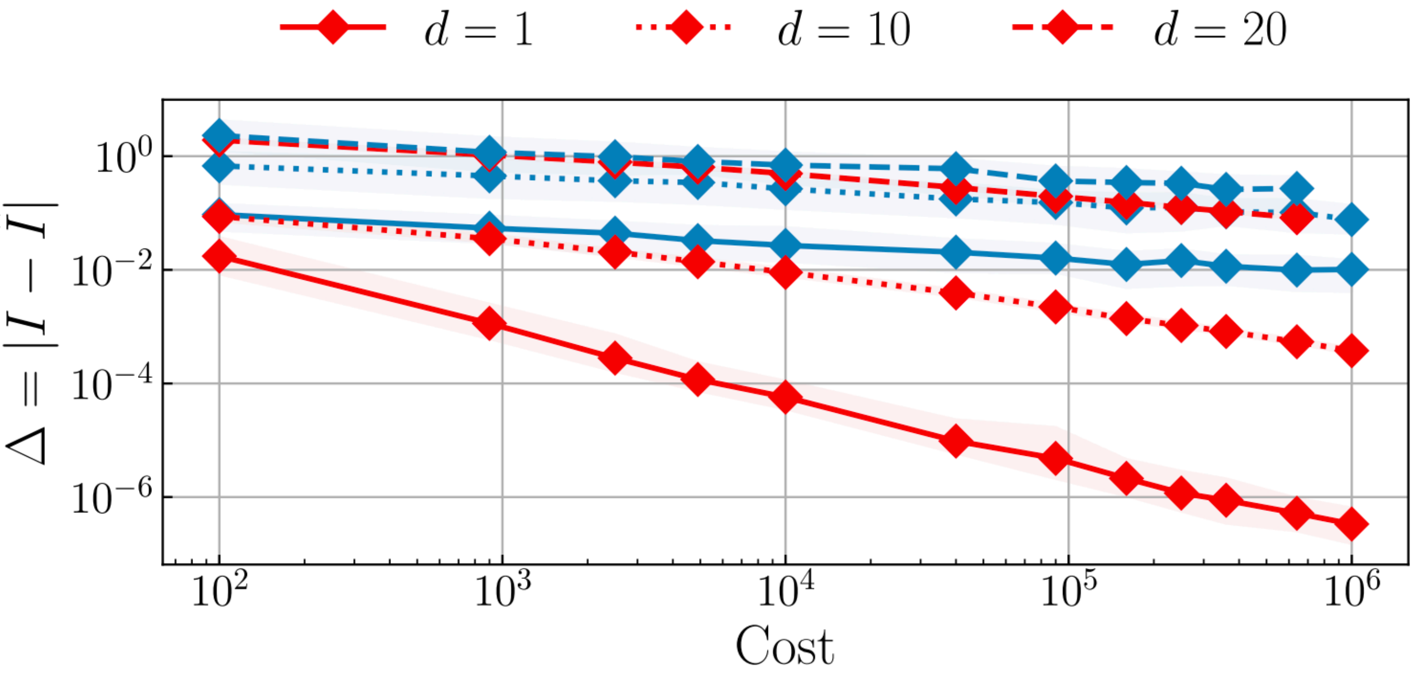

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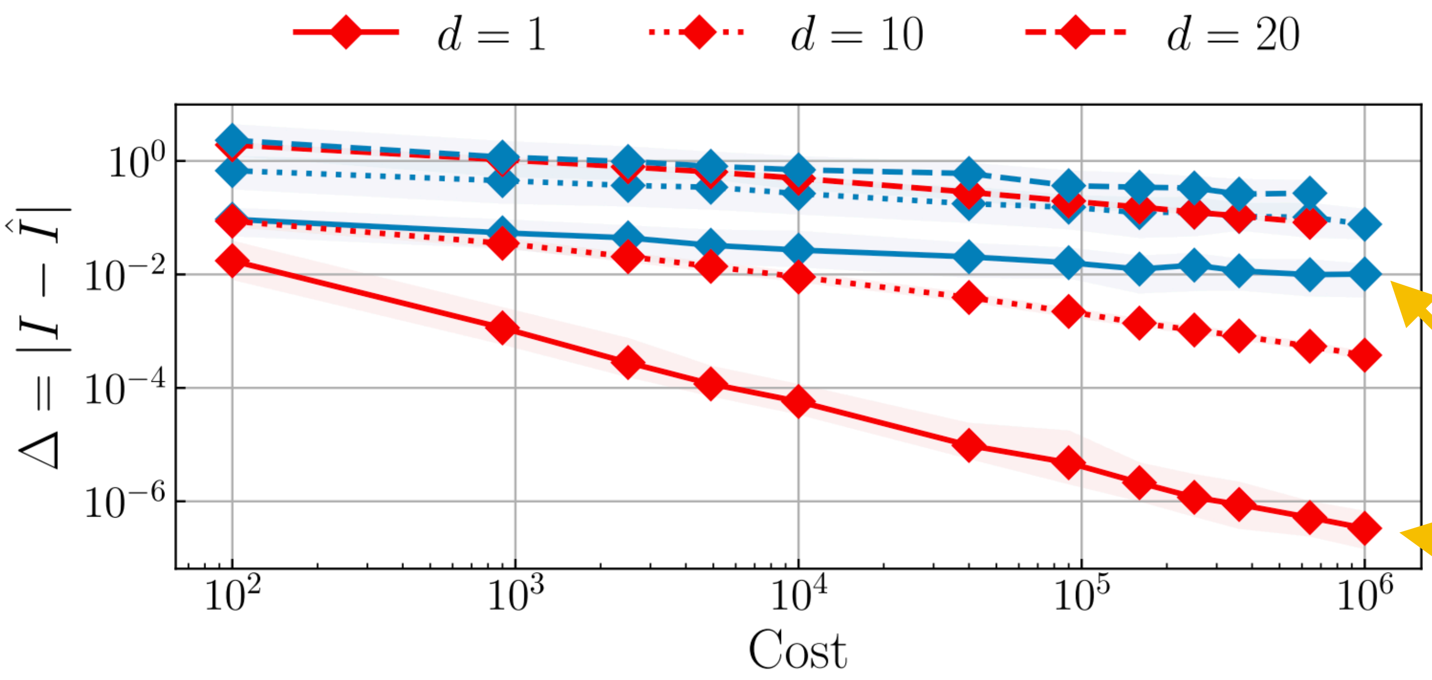

We do great in one dimension (as seen previously)

We suffer in high dimensions…

$$g(x,\theta) = \|x\|_2^{\frac{5}{2}} + \|\theta\|_2^{\frac{5}{2}}$$

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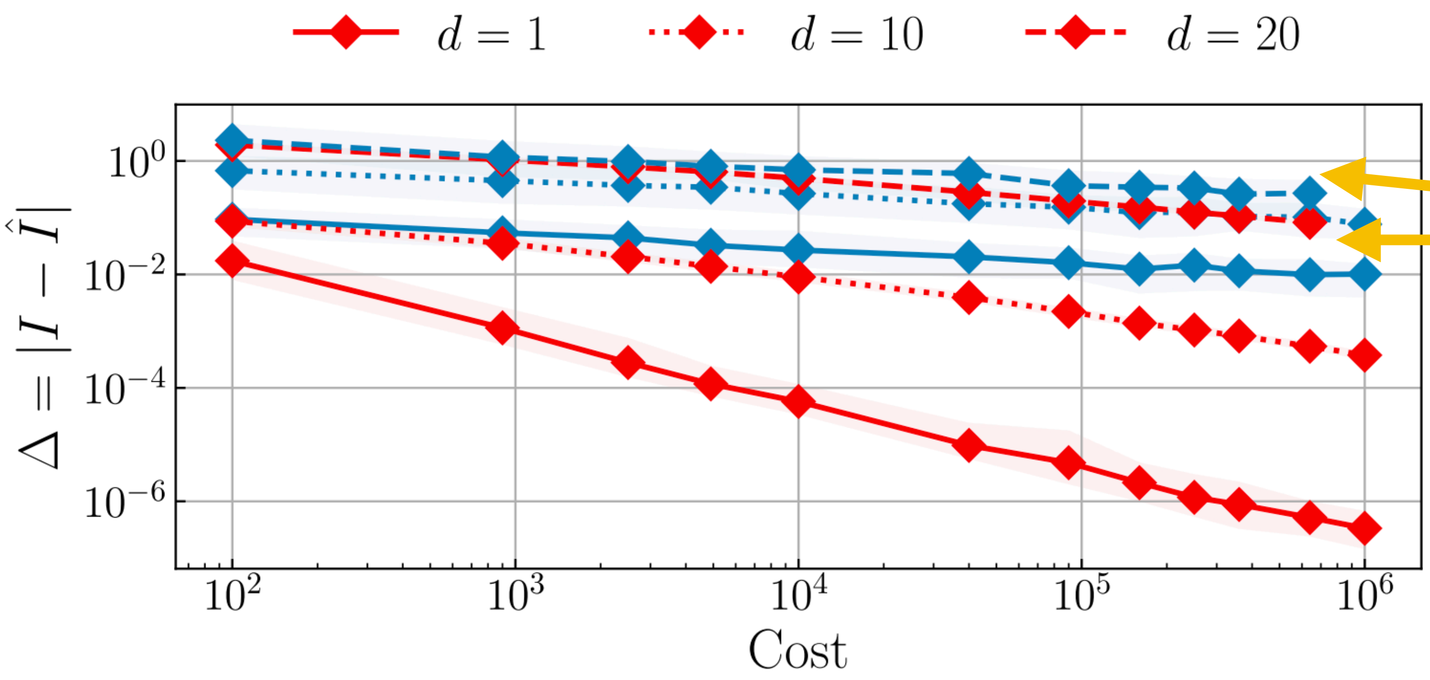
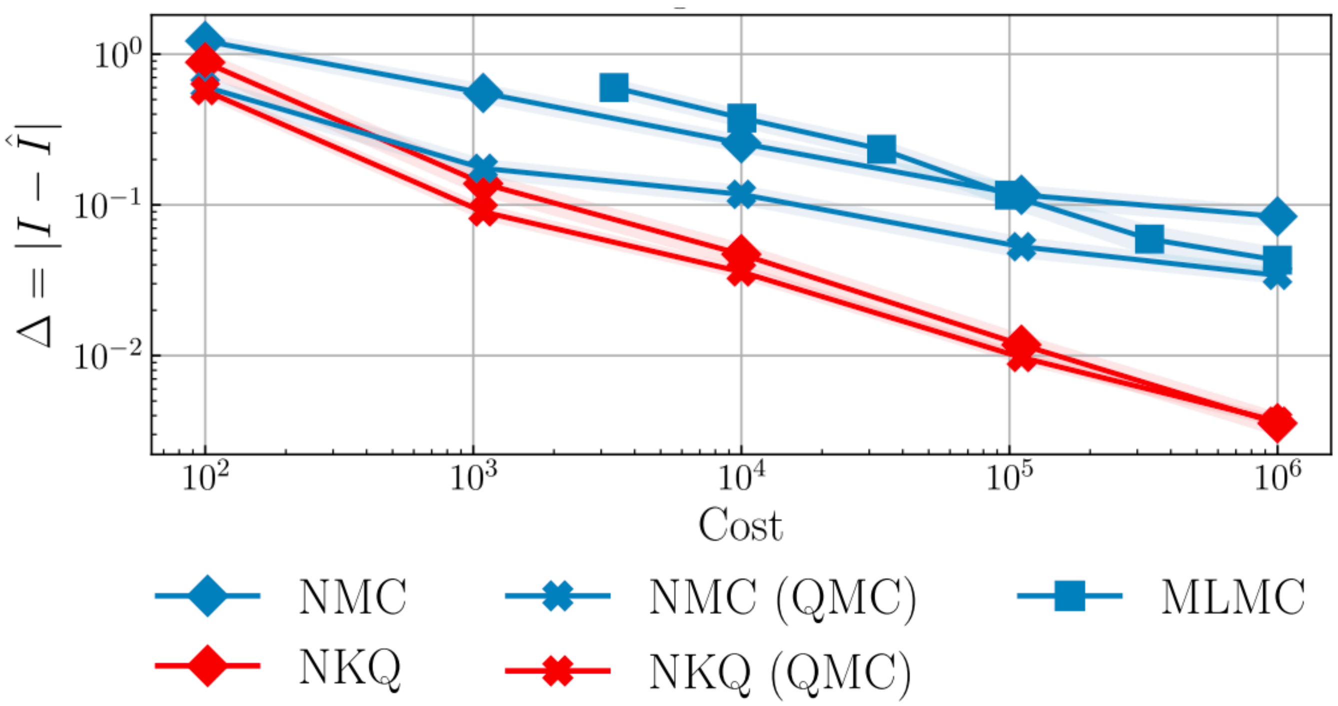


We do much worse in higher dimensions!

Option pricing



- **Problem:** Pricing of options; expected loss of portfolio in the presence of potential economic shock.

Chen, Z., Naslidnyk, M., Gretton, A., & Briol, F.-X. (2024). Conditional Bayesian quadrature. *Uncertainty in Artificial Intelligence*, 648–684.

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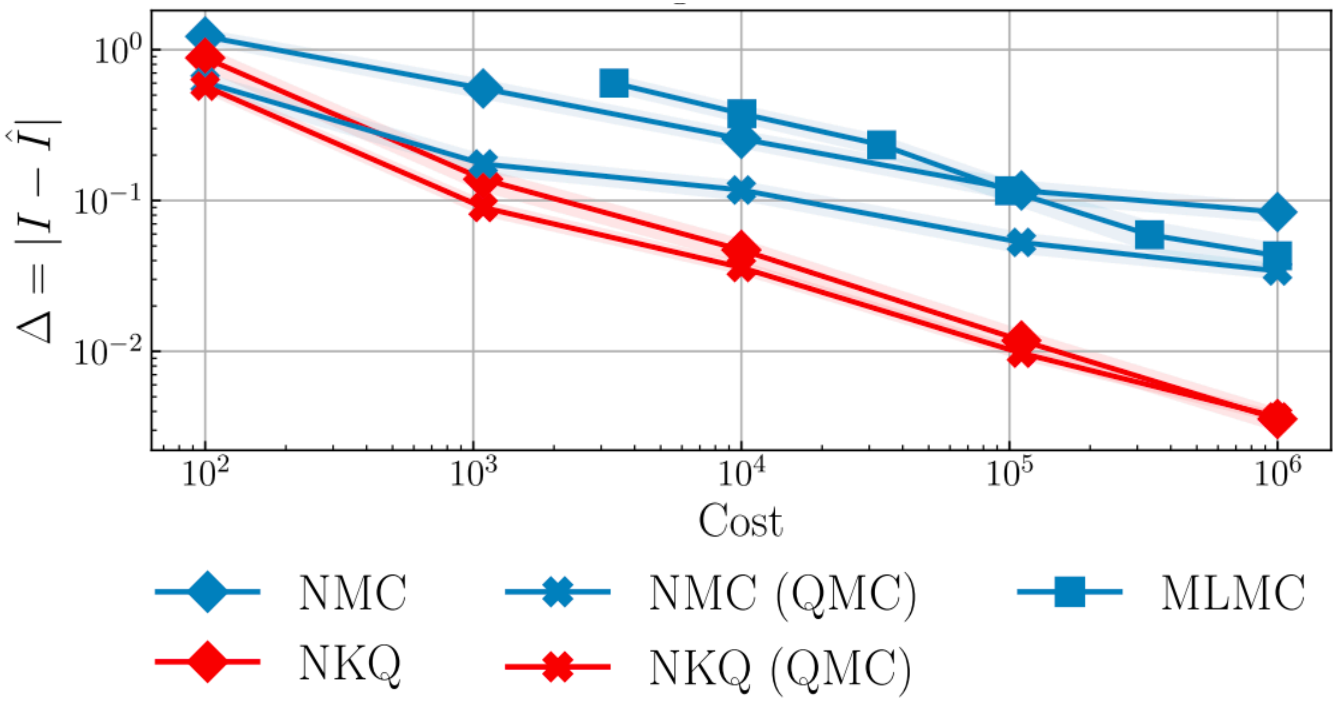

- **Problem:** Pricing of options; expected loss of portfolio in the presence of potential economic shock.
- Some of the assumptions are broken (unbounded domain, $f \notin C_b^2$)
- We used $k_{\mathcal{X}}$ and k_Θ with $s_{\mathcal{X}} = s_\Theta = 1$.

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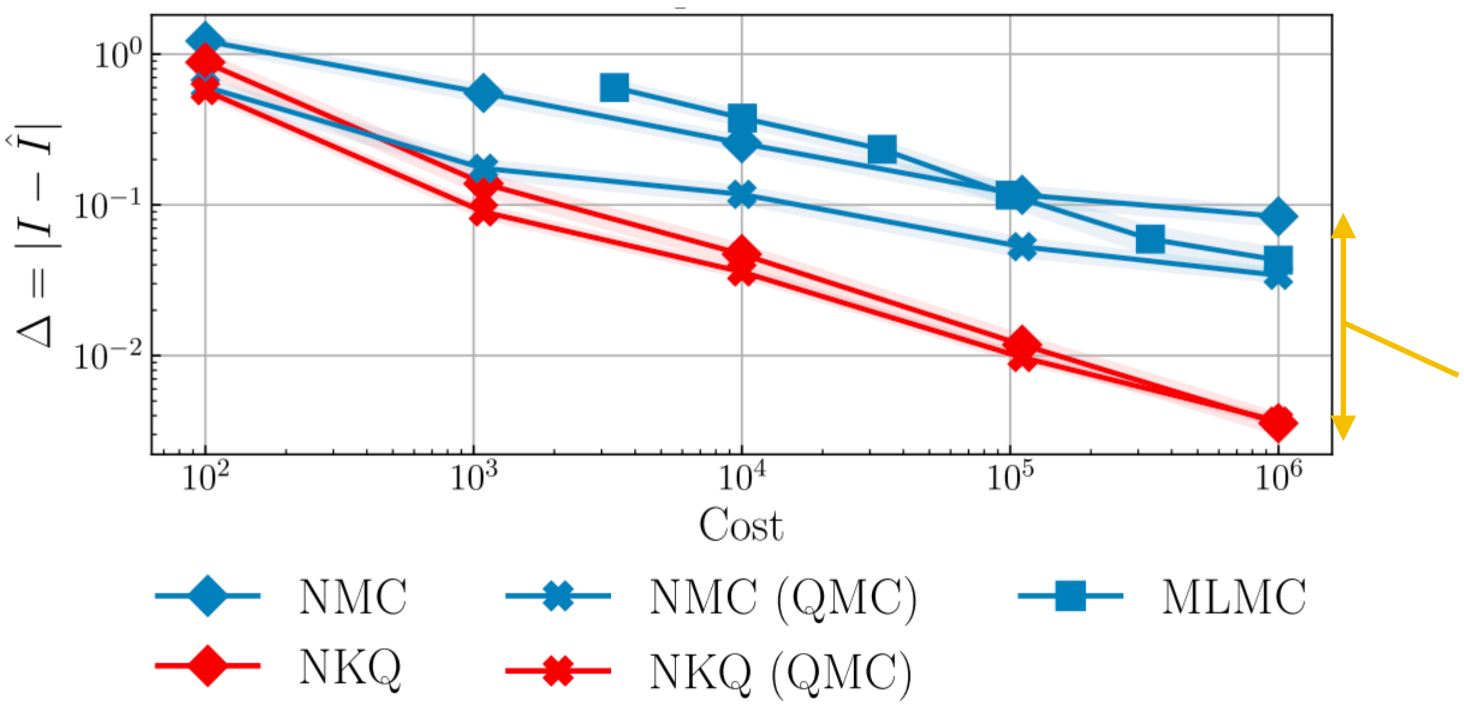

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Approx **100x smaller** error than NMC

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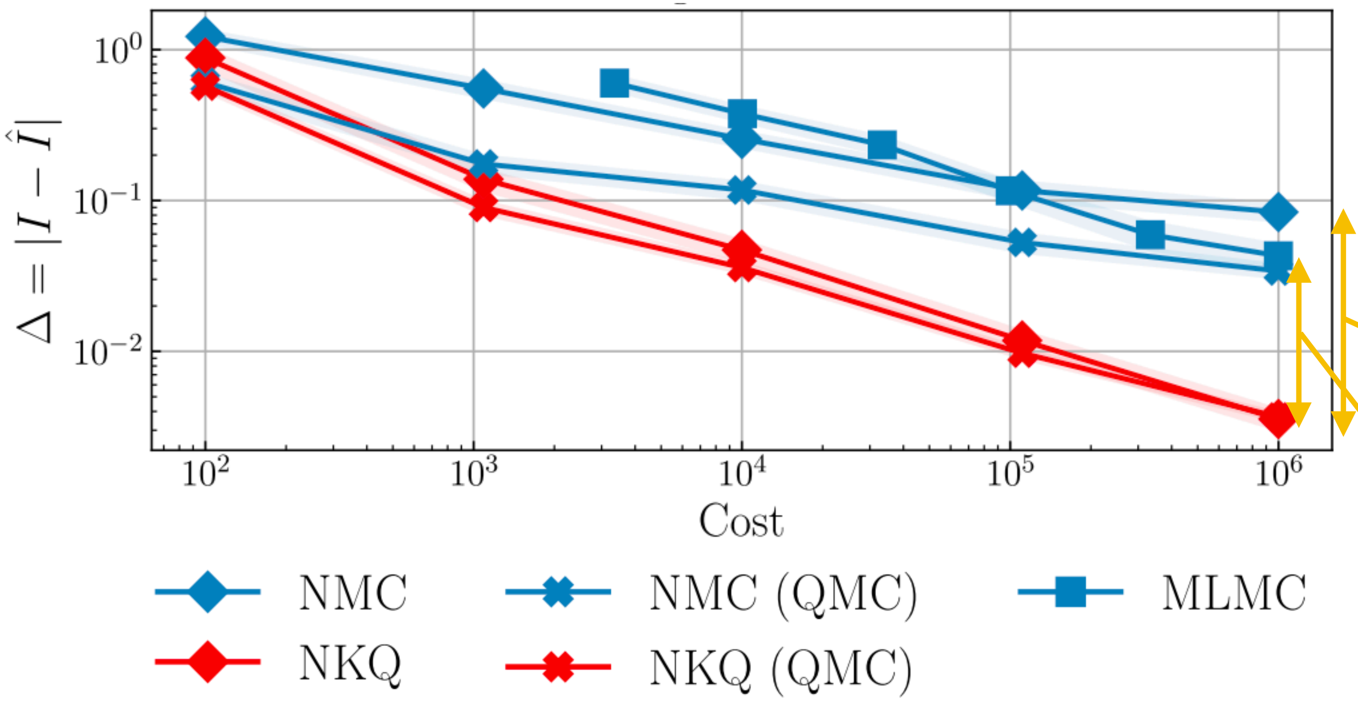

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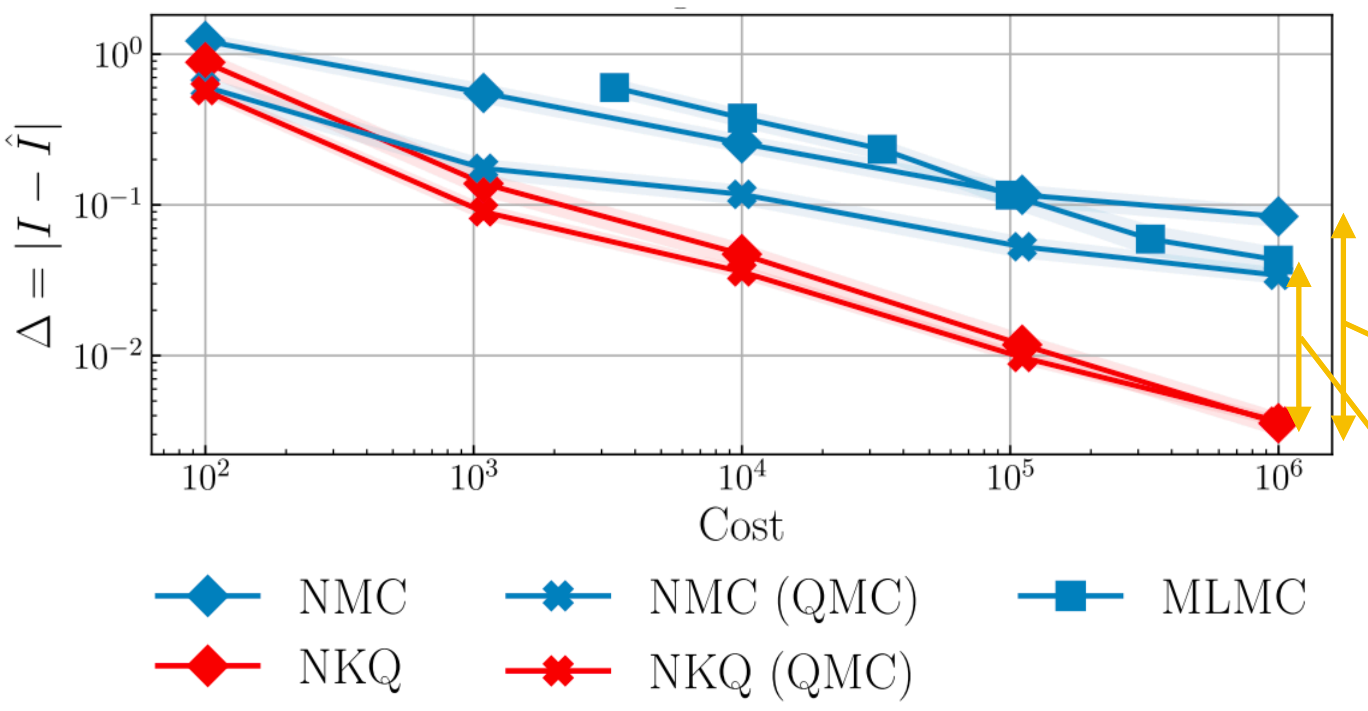

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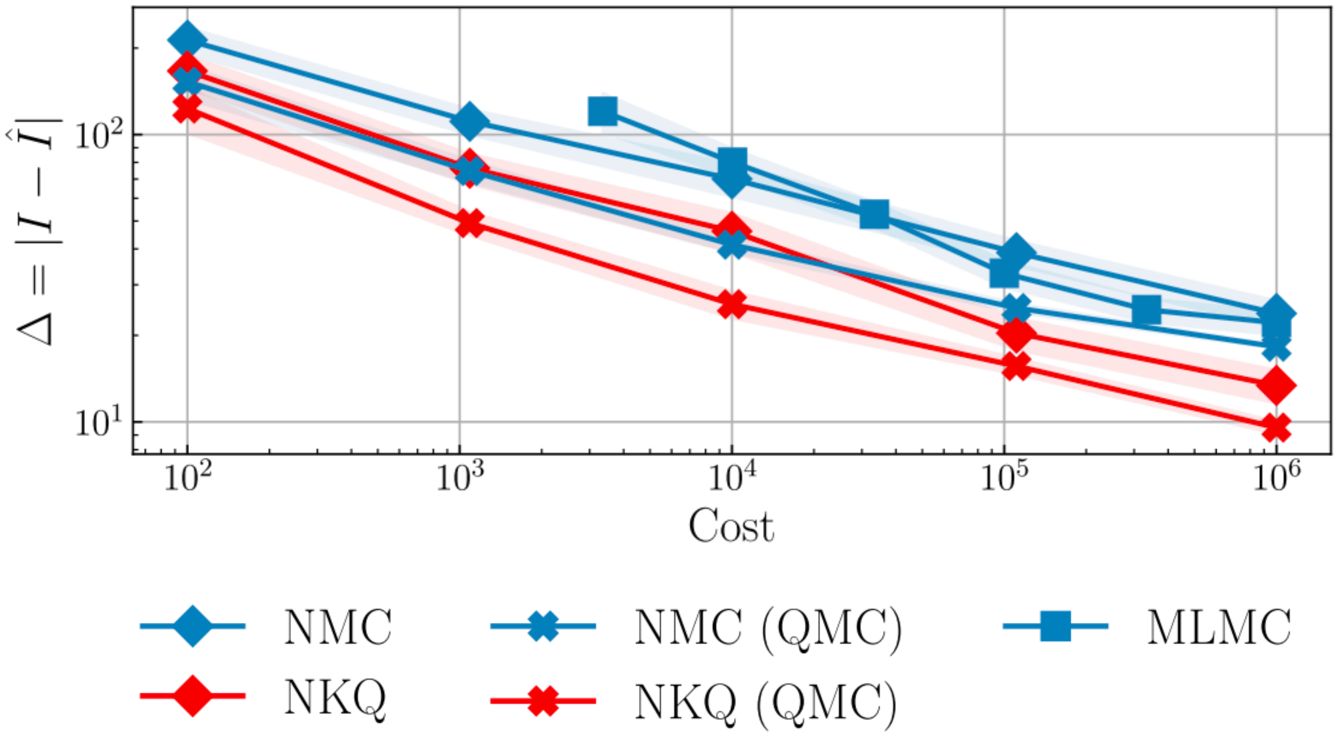
- We have Cost = $O(\Delta^{-r})$ and estimated:

- $\hat{r}_{\text{NMC}} = 2.97$ ($r_{\text{NMC}} = 3$)
- $\hat{r}_{\text{NKQ}} = 1.9$ ($r_{\text{NKQ}} = 2$)

Chen, Z., Naslidnyk, M., Gretton, A., & Briol, F.-X. (2024). Conditional Bayesian quadrature. *Uncertainty in Artificial Intelligence*, 648–684.

Health economics



- **Problem:** Computing the expected value of partial perfect information. QoI for deciding whether we want to collect measurements on more variables from patients.

- We use $s_{\mathcal{X}} = s_{\Theta} = \infty$.

Hironaka, T., Giles, M. B., Goda, T., & Thom, H. (2020). Multilevel Monte Carlo estimation of the expected value of sample information. *SIAM-ASA Journal on Uncertainty Quantification*, *8*(3), 1236–1259.

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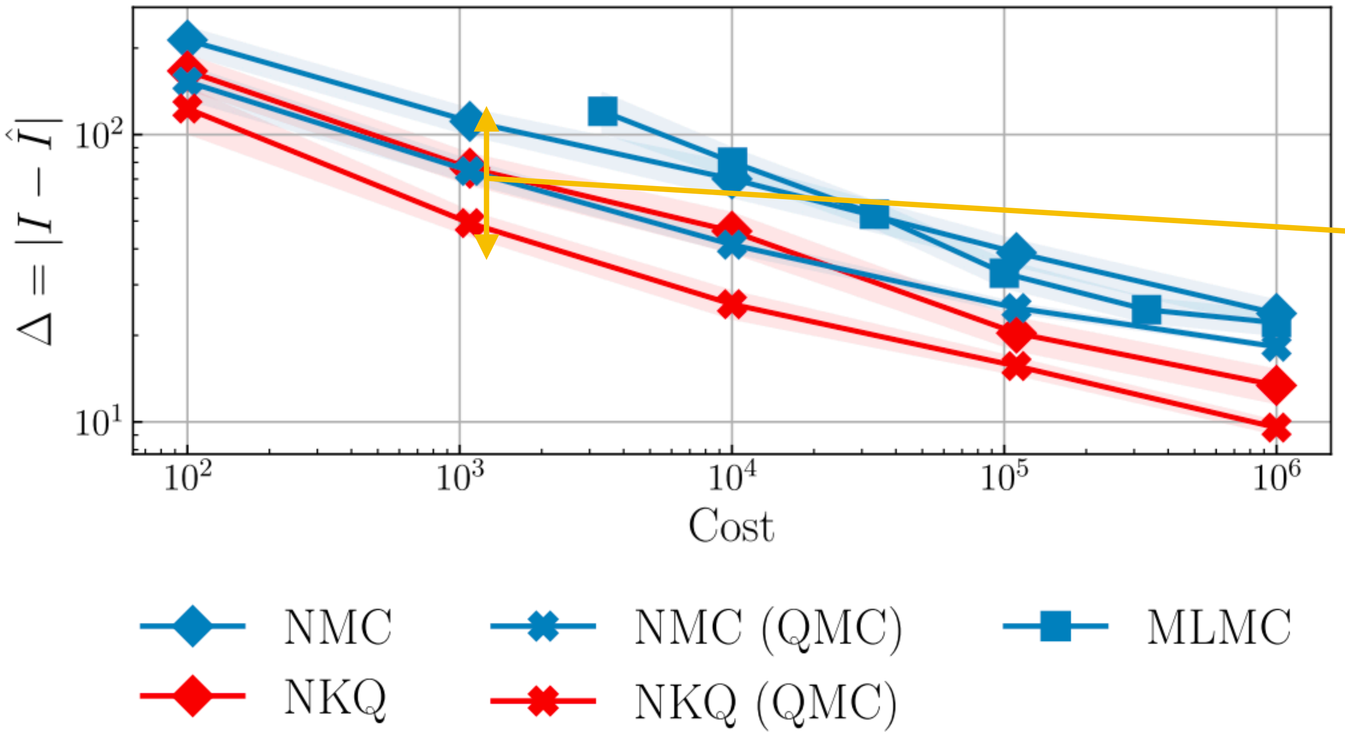

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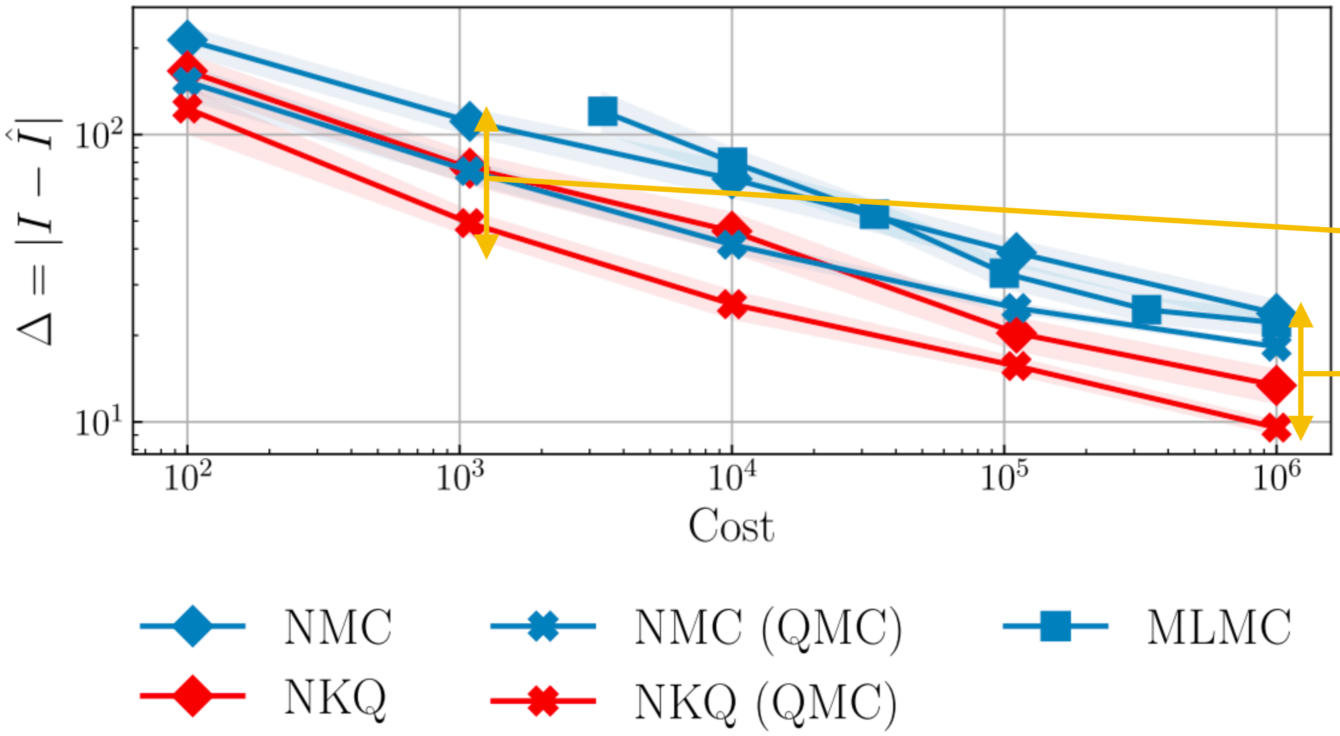

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Much smaller gains….

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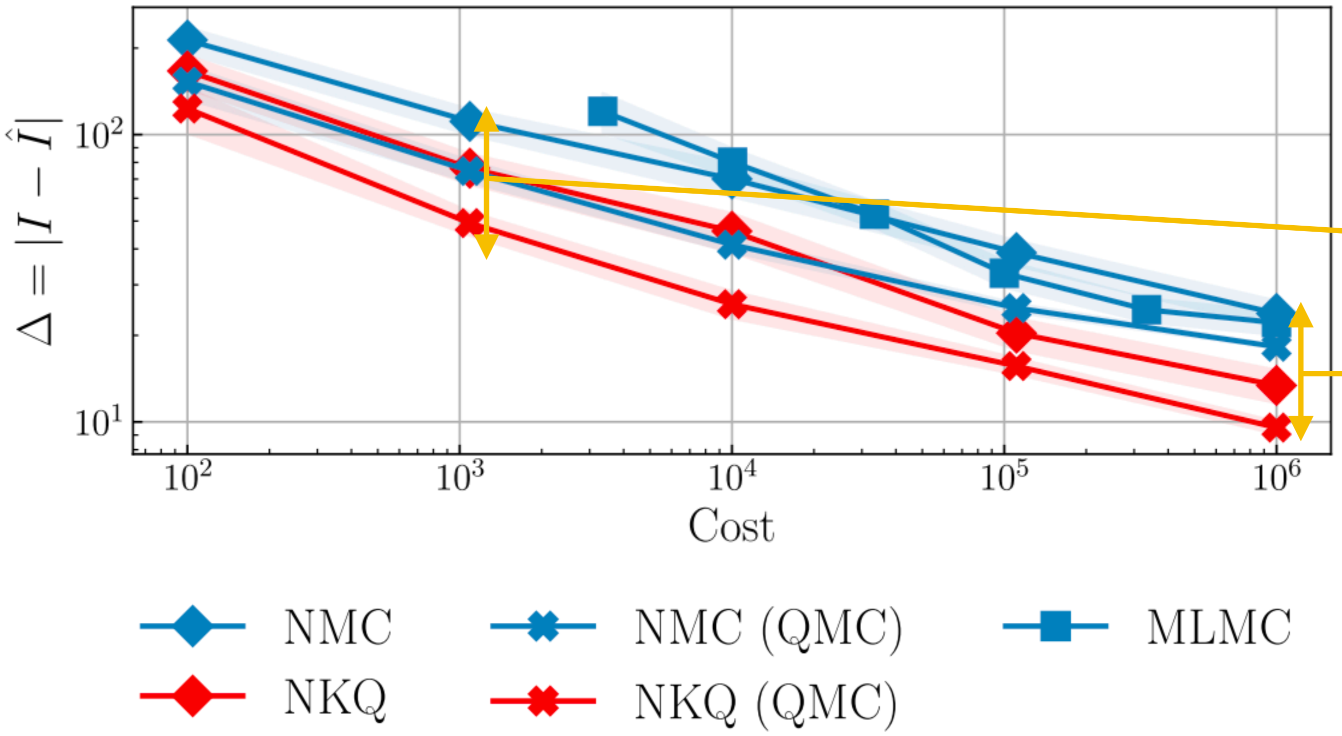

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Why not as good?

- The problem is high-dimensional:

$$d_{\mathcal{X}} = 17$$

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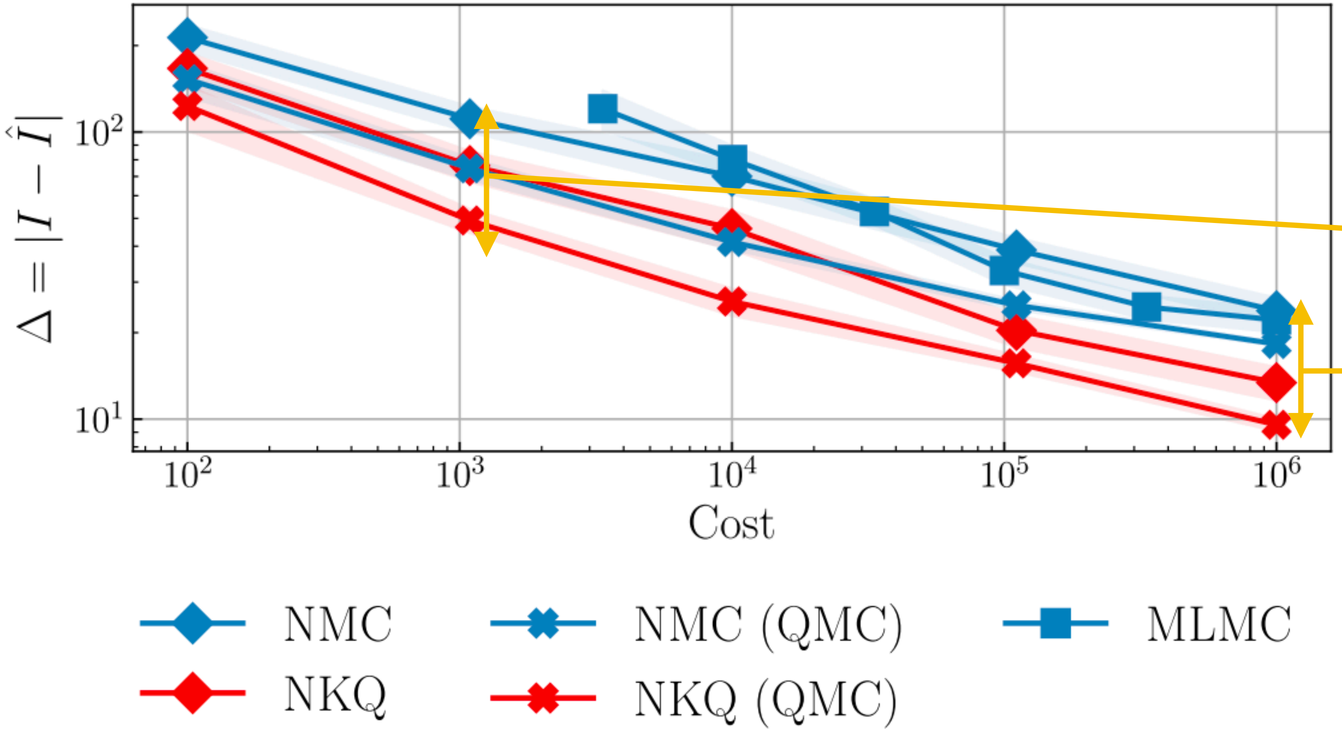

Approx **3x smaller** error than NMC

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We might still be very happy with 3x smaller error for small N & T!!

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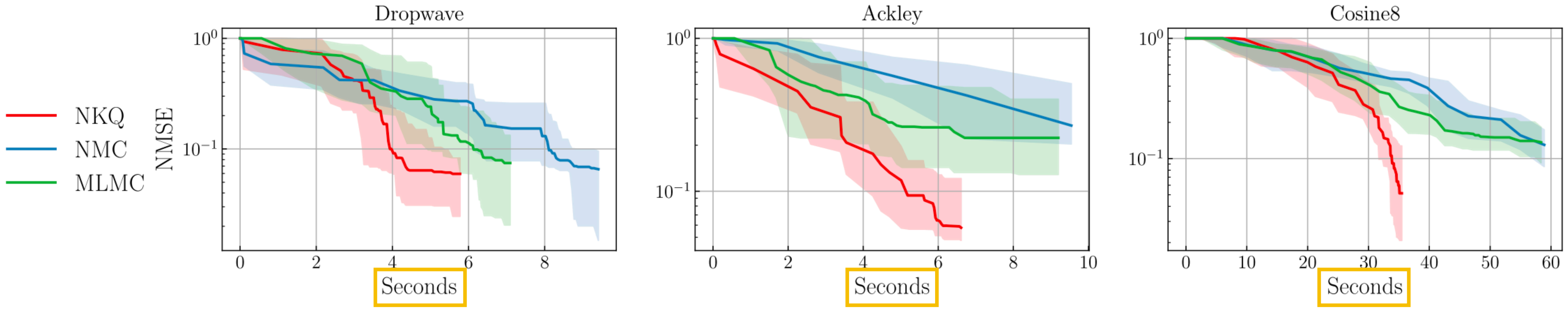
Look-ahead Bayesian optimisation



- **Problem:** Repeatedly computing and optimising acquisition function for 2-step look-ahead Bayesian optimisation. This requires compute a **very large number** of nested expectations.

Yang, S., Zankin, V., Balandat, M., Scherer, S., Carlberg, K., Walton, N., & Law, K. J. H. (2024). Accelerating look-ahead in Bayesian optimization: Multilevel Monte Carlo is all you need. *International Conference on Machine Learning*, 56722–56748.

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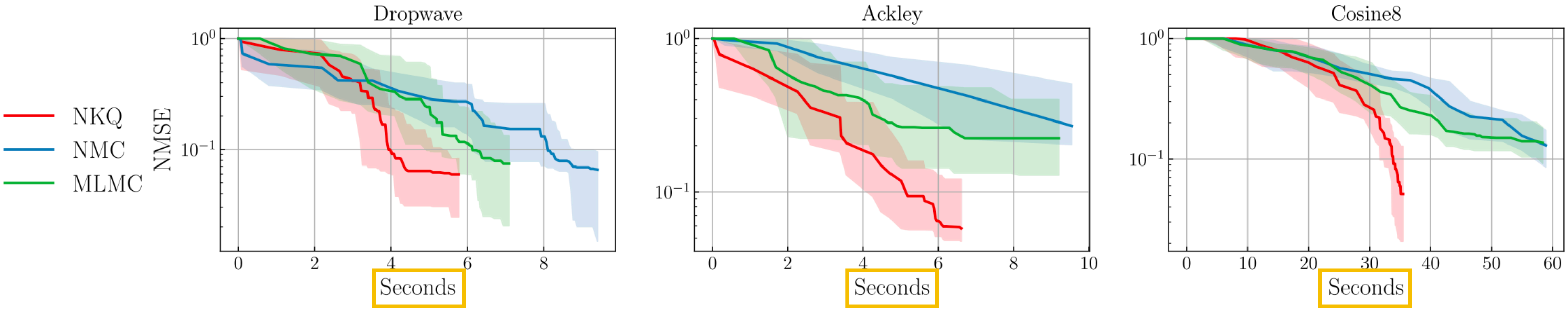

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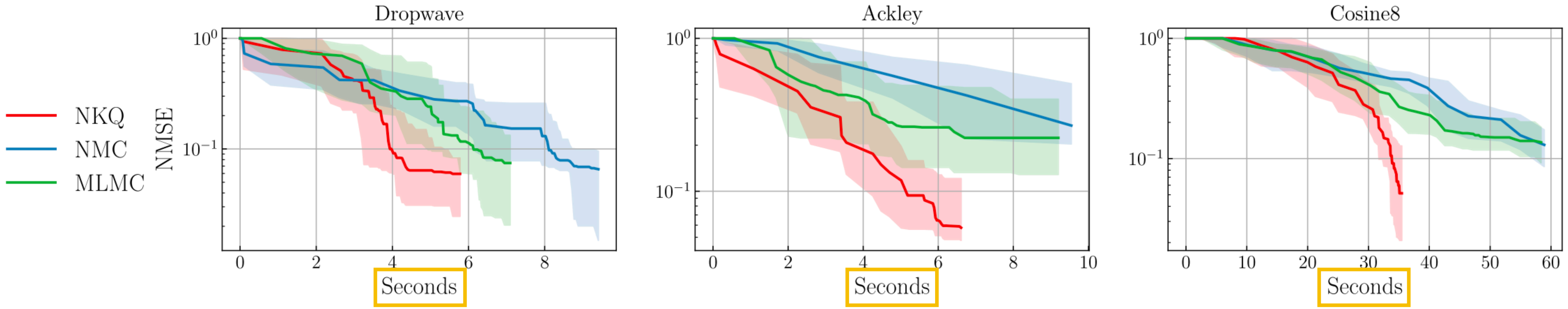

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- Cubic cost for NKQ only occurs once since the matrix inverses can be re-used (through change of variable trick).

Yang, S., Zankin, V., Balandat, M., Scherer, S., Carlberg, K., Walton, N., & Law, K. J. H. (2024). Accelerating look-ahead in Bayesian optimization: Multilevel Monte Carlo is all you need. *International Conference on Machine Learning*, 56722–56748.

Summary and future work

- **Summary:** New estimator whose cost is orders of magnitude smaller than competitors when the integrands are smooth and dimensions not too high:

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  - In-depth study of multilevel KQ approach?

Li, K., Giles, D., Karvonen, T., Guillas, S., & Briol, F.-X. (2023). Multilevel Bayesian quadrature. *International Conference on Artificial Intelligence and Statistics (with oral presentation)*, 1845–1868.

Any Questions?

Chen, Z., Naslidnyk, M., & Briol, F.-X. (2025). Nested expectations with kernel quadrature. a*rXiv:2502.18284*.