Deflated Multigrid Multilevel Monte Carlo

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STIMULATE
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Short recap

Short recap

Multigrid multilevel Monte Carlo for $\mathrm{tr}(A^{-1})$

The problem at hand is: $\mathrm{tr}(A^{-1})$. The method presented here works for any $f(A)$, in particular any $f(A) = (\Gamma A)^{-1}$: but we focus on $f(A) = A^{-1}$:

We start with the decomposition:

$$\mathrm{tr}(A^{-1}) = \sum_{\ell=1}^{L-1} \mathrm{tr}\left(\hat{P}_\ell A_\ell^{-1} \hat{R}_\ell - \hat{P}_{\ell+1} A_{\ell+1}^{-1} \hat{R}_{\ell+1}\right) + \mathrm{tr}(\hat{P}_L A_L^{-1} \hat{R}_L).$$

Why should this reduce the variance?

$$\mathbb{V}[x^H A^{-1} x] = \|\mathrm{offdiag}(A^{-1})\|_F^2 = \sum_{i=1}^{n} \sigma_i^{-2} - \sum_{i=1}^{n} |(A^{-1})_{ii}|^2$$

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A bit more specifically:

- two levels: $\mathrm{tr}(A_1^{-1}) = \mathrm{tr}(A_1^{-1}) - \mathrm{tr}(P_1 A_2^{-1} R_1) + \mathrm{tr}(P_1 A_2^{-1} R_1)$
- multilevel ($R_\ell P_\ell = I$):
  $\mathrm{tr}(A^{-1}) = \sum_{\ell=1}^{L-1} \mathrm{tr}\left(A_\ell^{-1} - P_\ell A_{\ell+1}^{-1} R_\ell\right) + \mathrm{tr}(A_L^{-1})$

We can connect this to inexact/approximate deflation:

$$A^{-1} = A^{-1}(I - \Pi) + A^{-1}\Pi$$

$$\Pi = \hat{U}_k(\hat{V}_k^* A \hat{U}_k)^{-1}\hat{V}_k^* A,\, \hat{U}_k, \hat{V}_k \in \mathbb{C}^{n\times k}$$

which is discussed in *Multigrid deflation for Lattice QCD* (Romero, Stathopoulos and Orginos), and already in Lüscher's local coherence paper.

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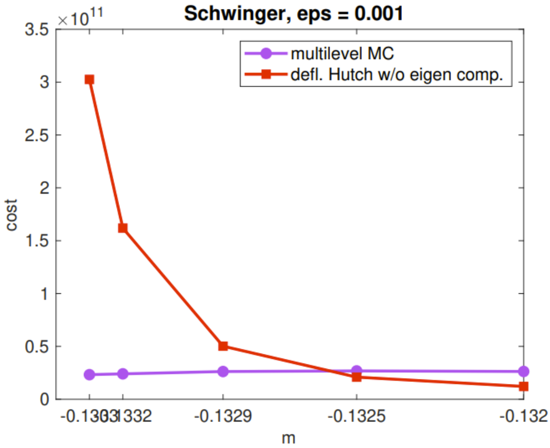
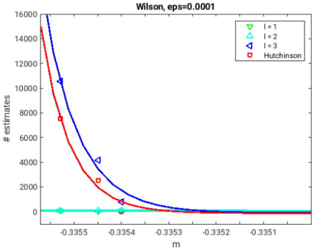
Short recap

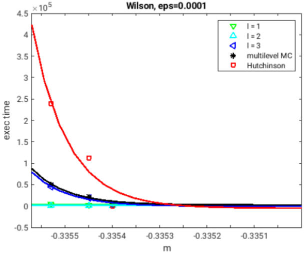
Multigrid multilevel Monte Carlo for $\mathrm{tr}(A^{-1})$



Some preliminary results in LQCD

Wilson: 64×32^3 (work in collaboration with Jose Jimenez-Merchan).
Twisted mass: 96×48^3.





	measurement	Mult. MC	Hutchinson
$\ell = 1$	# estimates	63	1164
	time (seconds)	17,010.0	221,160.0
$\ell = 2$	# estimates	172	-
	time (seconds)	15,480.0	-
$\ell = 3$	# estimates	903	-
	time (seconds)	9,030.0	-
$\ell = 4$	# estimates	7715	-
	time (seconds)	1,543.0	-
total	# estimates	-	1164
total	time (seconds)	43,063.0	221,160.0

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Skipping levels in multigrid multilevel Monte Carlo

Let's fully write a four-level expansion:

$$\operatorname{tr}(A^{-1}) = \operatorname{tr}\left(A_1^{-1} - P_1 A_2^{-1} R_1\right) + \operatorname{tr}\left(P_1 A_2^{-1} R_1 - P_1 P_2 A_3^{-1} R_2 R_1\right) + \operatorname{tr}\left(P_1 P_2 A_3^{-1} R_2 R_1 - P_1 P_2 P_3 A_4^{-1} R_3 R_2 R_1\right) + \operatorname{tr}\left(P_1 P_2 P_3 A_4^{-1} R_3 R_2 R_1\right)$$

Skip second level-difference:

$$\operatorname{tr}(A^{-1}) = \operatorname{tr}\left(A_1^{-1} - P_1 P_2 A_3^{-1} R_2 R_1\right) + \operatorname{tr}\left(P_1 P_2 A_3^{-1} R_2 R_1 - P_1 P_2 P_3 A_4^{-1} R_3 R_2 R_1\right) + \operatorname{tr}\left(P_1 P_2 P_3 A_4^{-1} R_3 R_2 R_1\right)$$

Then, reduce further:

$$\operatorname{tr}(A^{-1}) = \operatorname{tr}\left(A_1^{-1} - P_1 P_2 A_3^{-1} R_2 R_1\right) + \operatorname{tr}\left((A_3^{-1} - P_3 A_4^{-1} R_3)(R_2 R_1 P_1 P_2)\right) + \operatorname{tr}\left(A_4^{-1}(R_3 R_2 R_1 P_1 P_2 P_3)\right)$$

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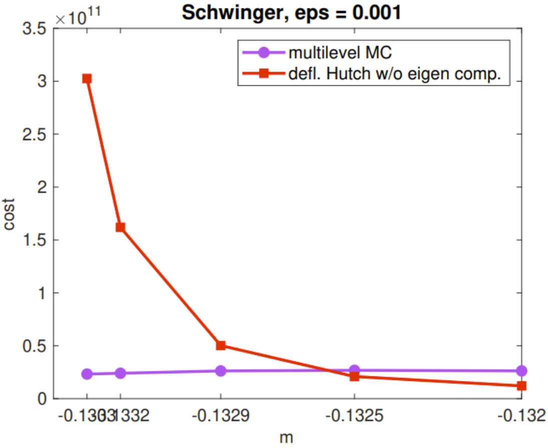
Exact deflation in multigrid multilevel Monte Carlo

Mostafa (talk on Th. @ 10:00) already talked about inexact deflation on top of multigrid multilevel Monte Carlo. Let's talk about exact deflation.



Exact deflation in MGMLMC

Deflating non-deflated modes

Exact deflation in "plain" Hutchinson:

$$\mathrm{tr}(A^{-1}) = A^{-1}(I - U_1 U_1^H) + \mathrm{tr}(U_1^H \Sigma_1^{-1} V_1)$$

In LQCD, to compute the singular vectors we can use:

$$A = U\Sigma V \Rightarrow Q = \Gamma_5 A$$

$$Q = X\Lambda X^H$$
$$\Rightarrow A = (\Gamma_5 X \mathrm{sign}(\Lambda))|\Lambda| V$$

Exact deflation in multigrid multilevel Monte Carlo:

instead of A, we have a more complicated operator to deflate from in multigrid multilevel Monte Carlo:

$$M_\ell = A_\ell^{-1} - P_\ell A_{\ell+1}^{-1} P_\ell^H$$

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Can we construct a symmetrized difference-level operator?

To do this easily, the multigrid hierarchy needs to be built via a Γ_5-compatible aggregation:

$$\Gamma_5^{\ell} P_{\ell} = P_{\ell} \Gamma_5^{\ell+1}, \quad P_{\ell}^H \Gamma_5^{\ell} = \Gamma_5^{\ell+1} P_{\ell}^H$$

and then:

$$\begin{aligned} J_{\ell} &= M_{\ell} \Gamma_5^{\ell} \\ &= A_{\ell}^{-1} \Gamma_5^{\ell} - P_{\ell} A_{\ell+1}^{-1} P_{\ell}^H \Gamma_5^{\ell} = Q_{\ell}^{-1} - P_{\ell} A_{\ell+1}^{-1} \Gamma_5^{\ell+1} P_{\ell}^H \\ &= Q_{\ell}^{-1} - P_{\ell} Q_{\ell+1}^{-1} P_{\ell}^H \end{aligned}$$

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Exact deflation in MGMLMC

Deflating non-deflated modes

$m_0 = -0.1320$, Schwinger. Single core, Python, laptop.

Method	exec. time	eigsolv. time
Hutch. + exact defl. (384)	1663.74	119.92
MGMLMC	2701.05	0.0
MGMLMC + exact defl. (32,32,32)	1067.77	1544.12
MGMLMC + exact defl. (32,32) + skip	530.26	948.35

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A (short) note on eigensolving

We need to compute large modes of the operator:

$$J_\ell = Q_\ell^{-1} - P_\ell Q_{\ell+1}^{-1} P_\ell^H$$

Done naively (as we have in our first tests with exact deflation), this is extremely expensive. It's probably better to transform the eigenproblem into a generalized Hermitian eigenproblem:

$$(Q_\ell^{-1} - P_\ell Q_{\ell+1}^{-1} P_\ell^H)v = \lambda v$$
$$\Rightarrow (I - Q_\ell P_\ell Q_{\ell+1}^{-1} P_\ell^H)v = \lambda Q_\ell v$$

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A (short) note on eigensolving

Using Jacobi-Davidson

$$(Q_\ell^{-1} - P_\ell Q_{\ell+1}^{-1} P_\ell^H) v = \lambda v$$

$$\Rightarrow (I - Q_\ell P_\ell Q_{\ell+1}^{-1} P_\ell^H) v = \lambda Q_\ell v$$

With the GHEP at hand, when using Jacobi-Davidson (which can be realized efficiently and scalably for Hermitian systems), we will need to apply the following operators at every iteration:

$$I - Q_\ell P_\ell Q_{\ell+1}^{-1} P_\ell^H$$

$$Q_\ell$$

and (very approximately e.g. 10^{-1}) solve a linear system with the operator:

$$(I - Q_\ell P_\ell Q_{\ell+1}^{-1} P_\ell^H) - \theta Q_\ell$$

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Thank you!

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