1D problem with recycling

December 2018

Table of content

- KL representation of the 1D lognormal diffusion field
- MCMC sampling of random modes
- Deflated CG (DCG) algorithm
- DCG for multiple right-hand-sides (DCGMRHS)
- DCG for multiple operators (DCGMO)

KL representation of a 1D lognormal field

- Let $\log \kappa(x,\theta) \sim G(x,\theta)$ where G has 0-mean and a square-exponential covariance $C(x,x') = \sigma^2 \exp(-(x-x')^2/2\ell)$.
- Consider the truncated KL representation of G:

$$\hat{G}(x,\theta) := \sum_{k=1}^{n_{\text{KL}}} \sqrt{\lambda_k} \phi_k(x) \xi_k(\theta) \text{ with } \xi := [\xi_1, \dots, \xi_{n_{\text{KL}}}]^T \sim \mathcal{N}(0, I_{n_{\text{KL}}})$$

where (λ_k, ϕ_k) are dominant solutions of the Fredholm integral eigenvalue problem stated by

$$\int_{\Omega} C(x, x')\phi(x')dx' = \lambda\phi(x).$$

We assume the eigenfunctions are orthonormal, i.e. $\langle \phi_i, \phi_j \rangle_{\Omega} = \delta_{ij}$.

• Resolution: Approximate solutions $(\hat{\lambda}_k, \hat{\phi}_k)$ are sought in the form

$$\hat{\phi}_k(x) = \sum_{j=1}^N d_j^k h_j(x)$$

for some $\{h_j\}_{j=1}^N$. From here on, different methods exist.

3 / 37

Nystrom's method

• Nystrom's method (Atkinson, 1997; Betz et al., 2014) relies on an approximation of the Fredholm integral by a quadrature

$$\sum_{j=1}^{N} w_j C(x, x_j) \hat{\phi}(x_j) = \hat{\lambda} \hat{\phi}(x) \text{ with weights } \{w_j\}_{j=1}^{N}$$

and integration points $\Omega_Q = \{x_j\}_{j=1}^N$. Solutions of the form $(\hat{\lambda}, y)$ with $y = [\hat{\phi}(x_1), \dots, \hat{\phi}(x_N)]^T$ are obtained by solving

$$\sum_{j=1}^{N} w_j C(x_i, x_j) \hat{\phi}(x_j) = \hat{\lambda} \hat{\phi}(x_i) \text{ for } i = 1, \dots, N$$

equivalently recast in $CWy = \hat{\lambda}y$ where $C_{ij} = C(x_i, x_j)$ and $W_{ij} = \delta_{ij}w_j$.

• To ensure $\hat{\lambda}_k > 0$, we write $W^{1/2}CW^{1/2}W^{1/2}y = \hat{\lambda}W^{1/2}y$ and solve

$$By^* = \hat{\lambda}y^*$$

instead, with $B = W^{1/2}CW^{1/2}$ and s.t. $y = W^{-1/2}y^*$.

Nystrom's method

• Denote the most dominant solutions of $By^* = \hat{\lambda}y^*$ by $\{(\hat{\lambda}_k, y_k^*)\}_{k=1}^{n_{\text{KL}}}$ and let $Y = W^{-1/2}[y_1^*, \dots, y_{n_{\text{KL}}}^*]$. Then, we have

$$\hat{\phi}_k(x) = \hat{\lambda}_k^{-1} \sum_{j=1}^N w_j C(x, x_j) \hat{\phi}_k(x_j) \text{ for } 1 \le k \le n_{\text{KL}}$$

so that we can approximately sample $\hat{G}(x,\theta)$ from

$$\sum_{k=1}^{n_{\text{KL}}} \hat{\lambda}_k^{1/2} \hat{\phi}_k(x) \xi_k(\theta) = \sum_{k=1}^{n_{\text{KL}}} \sum_{j=1}^N w_j \hat{\lambda}_k^{-1/2} C(x, x_j) \hat{\phi}_k(x_j) \xi_k(\theta).$$

• We can then sample $\hat{G}(\{x^{(s)}\}_{s=1}^{n_s}, \theta) = [\hat{G}(x^{(1)}, \theta), \dots, \hat{G}(x^{(n_s)}, \theta)]^T$ by

$$\hat{G}(\{x^{(s)}\}_{s=1}^{n_s}, \theta) \approx \tilde{C}WY\Lambda^{-1/2}\xi(\theta) = \tilde{C}W^{1/2}Y^*\Lambda^{-1/2}\xi(\theta) \text{ with } \xi \sim \mathcal{N}(0, I_{n_{\text{KL}}})$$
where $\Lambda_{ij} = \delta_{ij}\hat{\lambda}_j$ and $\tilde{C}_{sj} = C(x^{(s)}, x_j)$.

• In the special case $\{x^{(s)}\}_{s=1}^{n_s} = \Omega_Q$, we have $\tilde{C} = C$ and

$$\hat{G}(\Omega_Q, \theta) \approx Y \Lambda^{1/2} \xi(\theta) = W^{-1/2} Y^* \Lambda^{1/2} \xi(\theta).$$

Galerkin projection

• Given a set of basis functions $\{h_j\}_{j=1}^N$, approximate solutions to the Fredholm integral equation are sought in the form $\hat{\phi}(x) = \sum_{j=1}^N d_j h_j(x)$, leading up to

$$\int_{\Omega} C(x, x') \hat{\phi}(x') dx' = \hat{\lambda} \hat{\phi}(x) + r(x)$$

with a residual $r(x) = \sum_{j=1}^{N} d_j \left[\int_{\Omega} C(x, x') h_j(x') dx' - \hat{\lambda} h_j(x) \right]$.

• Approximate solutions $(\hat{\lambda}, \{d_j\}_{j=1}^N)$ are obtained upon enforcing orthogonality as follows,

$$\int_{\Omega} \sum_{i=1}^{N} d'_{i} h(x) r(x) dx = 0 \quad \forall \quad \{d'_{i}\}_{i=1}^{N}$$

equivalently stated by $Bd = \hat{\lambda} Md$ where $d = [d_1, \dots, d_N]^T$,

$$B_{ij} = \int_{\Omega} C(x, x') h_i(x') dx' h_j(x) dx \text{ and } M_{ij} = \int_{\Omega} h_i(x') dx' h_j(x) dx.$$
_{6/37}

Galerkin projection

• Denote the most dominant solutions of $Bd = \hat{\lambda}Md$ by $\{(\hat{\lambda}_k, d^{(k)}\}_{k=1}^{n_{\rm KL}}$ and let $D = [d^{(1)}, \dots, d^{(n_{\rm KL})}]$. Then, we have

$$\hat{\phi}_k(x) = \sum_{j=1}^N d_j^{(k)} h_j(x) \text{ for } 1 \le k \le n_{\text{KL}}$$

so that we can approximately sample $\hat{G}(x,\theta)$ from

$$\sum_{k=1}^{n_{\text{KL}}} \hat{\lambda}_k^{1/2} \hat{\phi}_k(x) \xi_k(\theta) = \sum_{k=1}^{n_{\text{KL}}} \sum_{j=1}^{N} \hat{\lambda}_k^{1/2} d_j^{(k)} h_j(x) \xi_k(\theta).$$

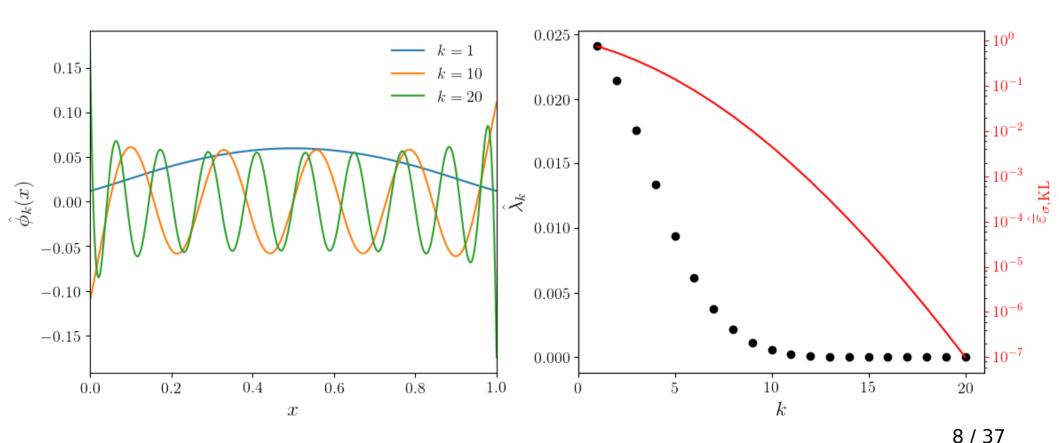
• We can then sample $\hat{G}(\{x^{(s)}\}_{s=1}^{n_s}, \theta) = [\hat{G}(x^{(1)}, \theta), \dots, \hat{G}(x^{(n_s)}, \theta)]^T$ by

$$\hat{G}(\{x^{(s)}\}_{s=1}^{n_s}, \theta) \approx HD\Lambda^{1/2}\xi(\theta) \text{ with } \xi \sim \mathcal{N}(0, I_{n_{\text{KL}}})$$

where $\Lambda_{ij} = \delta_{ij} \hat{\lambda}_j$ and $H_{sj} = h_j(x^{(s)})$.

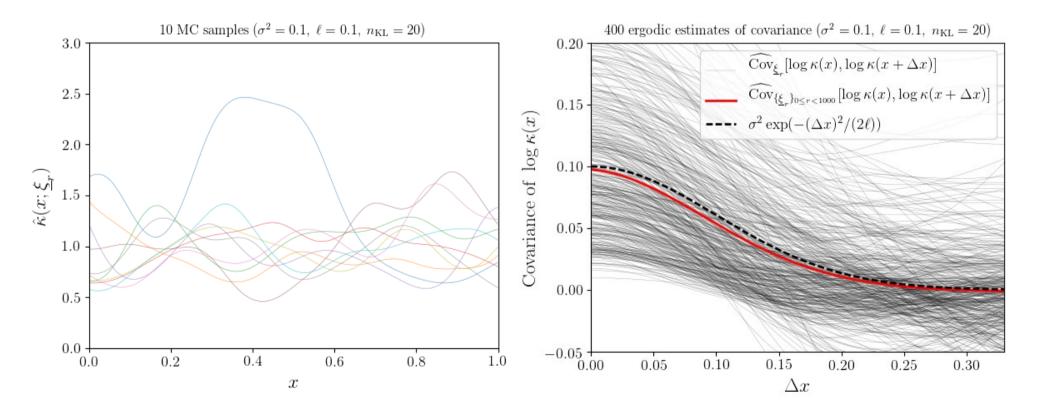
KL representation of a 1D lognormal field

- Consider P0 finite elements for $\Omega=[0,1]$ with N=500 , $n_{\rm KL}=20$, $\sigma^2=0.1$ and $\ell=0.1$.
- We denote the mean error variance by $\overline{\varepsilon}_{\sigma,\mathrm{KL}} = 1 |\Omega|^{-1} \sum_{k=1}^{n_{\mathrm{KL}}} \frac{\lambda_k}{\sigma^2}$.



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MCMC sampling of ξ

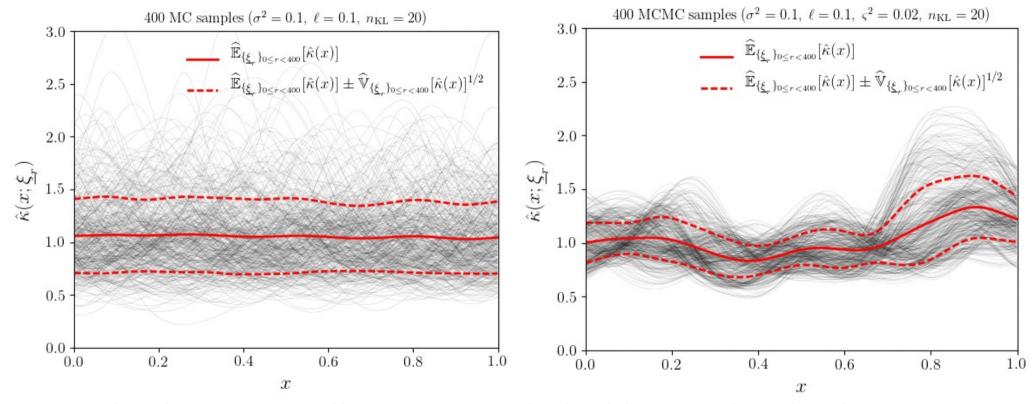
- Motivation: Increase similarity between consecutively sampled realizations in order to eventually recycle information from one solved linear system to another.
- Given a realization $\xi^{(r)}$, candidates for $\xi^{(r+1)}$ are proposed as samples of $\chi^{(r+1)} \sim \xi^{(r)} + \varsigma \mathcal{N}(0, I_{n_{\text{KL}}})$ so that the ratio of proposal densities $q(\xi^{(r)}|\chi^{(r+1)})/q(\chi^{(r+1)}|\xi^{(r)})$ amounts to 1.
- A proposed state $\chi^{(r+1)}$ is then accepted with probability

$$\alpha(\xi^{(r)}, \chi^{(r+1)}) = \min\left\{\frac{f(\chi^{(r+1)})}{f(\xi^{(r)})}, 1\right\} = \min\left\{\exp(\|\xi^{(r)}\|_2^2 - \|\chi^{(r+1)}\|_2^2), 1\right\}$$

• We denote by $\{\xi^{(s)}\}_{s=1}^{\nu}$ the sequence of accepted candidates sampled after $\xi^{(1)} \sim \mathcal{N}(0, I_{n_{\text{KL}}})$.

How do we pick ς^2 ?

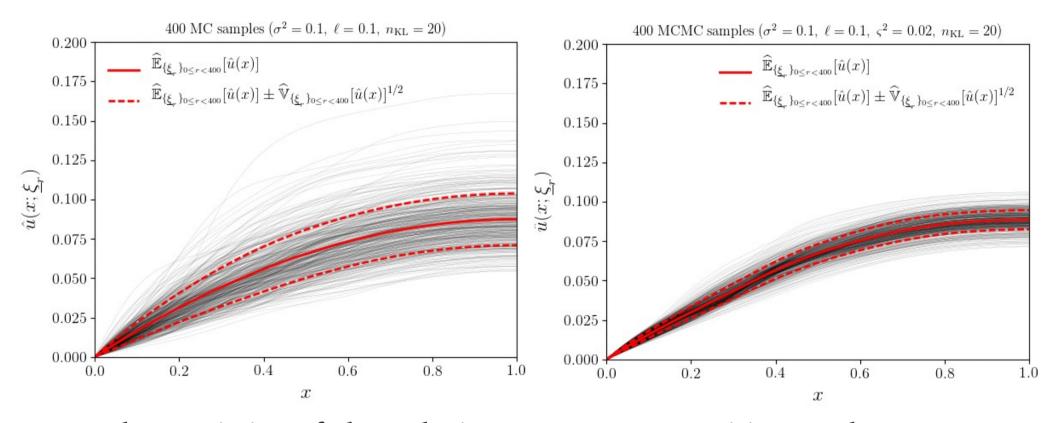
• Let's compare subsequences of realizations obtained by MCMC with realizations obtained by MC:



- Clearly, MCMC allows to sample highly correlated subsequences.
- For a specific number of realizations, how should we pick ς^2 ? Should we run several independent chains?

How do we pick ς^2 ?

• Considering a FE discretization with P1 elements and homogeneous Dirichlet-Neumann BC, we obtain:



• The statistics of the solution are not as sensitive to the sampling method as those of the coefficient field.

Deflated CG (DCG) in a nutshell

• Given a basis $W \in \mathbb{R}^{n \times k}$ with $k \ll n$ and an initial guess x_0 s.t.

$$r_0 := b - Ax_0 \perp \operatorname{span}\{W\} =: \mathcal{W},$$

• Deflated CG (Saad et al., 2000) builds a sequence of iterates $\{x_j\}_{j=1,2,...}$ s.t.

$$x_j - x_0 \in \mathcal{W} \oplus \mathcal{K}_j(A, r_0) =: \mathcal{K}_{k,j}(A, W, r_0),$$

and $r_j := b - Ax_j \perp \mathcal{W} \oplus \mathcal{K}_j(A, r_0).$

• DCG (A, W, x_0) // x_0 is s.t. $r_0 := b - Ax_0 \perp \text{span}\{W\}$ Solve $W^T A W \hat{\mu}_0 = W^T A r_0$ for $\hat{\mu}_0$ and set $p_0 = r_0 - W \hat{\mu}_0$ For j = 1, ..., m, Do: $\alpha_{j-1} = r_{j-1}^T r_{j-1} / p_{j-1}^T A p_{j-1}$ $x_j = x_{j-1} + \alpha_{j-1} p_{j-1}$ $r_j = r_{j-1} - \alpha_{j-1} A p_{j-1}$ $\beta_{j-1} = r_j^T r_j / r_{j-1}^T r_{j-1}$ Solve $W^T A W \hat{\mu}_j = W^T A r_j$ for $\hat{\mu}_j$ $p_j = \beta_{j-1} p_{j-1} + r_j - W \hat{\mu}_j$

DCG - Why "deflation"?

ullet Consider the oblique projector along ${\mathcal W}$ given by

$$H = I_n - W(W^T A W)^{-1} (A W)^T.$$

• The solution to the original system Ax = b is decomposed into

$$x = \underbrace{(I_n - H)x}_{x_1 \in \mathcal{W}} + \underbrace{Hx}_{x_2 \in \mathcal{W}^{\perp}}$$

where $x_1 = W\hat{x}_1$ in which \hat{x}_1 is solution of the reduced system

$$W^T A W \hat{x}_1 = W^T b$$

and $AHx = H^TAx = H^TAHx$ so that $x_2 = H\hat{x}_2$ where \hat{x}_2 is solution of a deflated, or nearly deflated system

$$H^T A H \hat{x}_2 = H^T b,$$

still consistent, and solvable by CG as long as solved with an initial residual in \mathcal{W}^{\perp} .

DCG - Deflation and convergence

• The sequence of iterates $\{x_j\}_{j=1,2,...}$ obtained by CG to solve the original system Ax = b with an initial guess x_0 admits

$$||x_j - x||_A \le 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1}\right)^j ||x_0 - x||_A$$

• On the other hand, the iterates obtained by CG applied to the deflated system $H^TAH\hat{x}_2 = H^Tb$ admit the following bound:

$$||x_j - \hat{x}_2||_A \le 2 \left(\frac{\sqrt{\kappa_{eff}(H^T A H)} - 1}{\sqrt{\kappa_{eff}(H^T A H)} + 1} \right)^{\jmath} ||x_0 - \hat{x}_2||_A$$

• The objective is then to find a projector H, or the basis of a deflation space \mathcal{W} , such that H^TAH is effectively better conditioned than A.

DCG - How to deflate?

- Let $\{u_i\}_{i=1,...,n}$ be the eigenvectors respectively associated with the eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ of A so that $\kappa(A) = \lambda_n/\lambda_1$.
- If the basis $W = [w_1, \dots, w_k]$ consists of the k eigenvectors of A associated with the least dominant eigenvalues λ_1 through λ_k , an effective conditioning number $\kappa_{eff}(H^TAH) = \lambda_n/\lambda_{k+1}$ is obtained.
- On the other hand, if the basis W consists of approximations of these k least dominant eigenvectors, we expect to obtain $\kappa(H^TAH) \approx \lambda_n/\lambda_{k+1}$.
- (Alternatively, W could be constructed solely of most dominant eigenvectors, or of both least and most dominant eigenvectors.)

DCG - Approximating eigenpairs of A

- Finding an approximation of an eigenpair (λ_i, u_i) of A can be done by searching an approximation of (λ_i^{-1}, u_i) for A^{-1} .
- Let $(\tilde{\lambda}_i^{-1}, y_i)$ denote an eigenpair approximation of A^{-1} obtained by the following harmonic projection:

$$y_i \in A\mathcal{K}_{k,\ell}(A, W, r_0),$$
$$A^{-1}y_i - \tilde{\lambda}_i^{-1}y_i \perp A\mathcal{K}_{k,\ell}(A, W, r_0)$$

where $\mathcal{K}_{k,\ell}(A,W,r_0)$ admits a basis $Z=[W,V_\ell]$, so that $y_i=AZ\tilde{y}_i$ and the orthogonality condition becomes

$$(AZ)^{T}(A^{-1}(AZ\tilde{y}_{i}) - \tilde{\lambda}_{i}^{-1}(AZ\tilde{y}_{i})) = 0,$$

$$Z^{T}AZ\tilde{y}_{i} - \tilde{\lambda}_{i}^{-1}(AZ)^{T}AZ\tilde{y}_{i} = 0.$$

• Hence, an approximate eigenpair $(\tilde{\lambda}_i, AZ\tilde{y}_i)$ of A is obtained when solving for a pair $(\tilde{\lambda}_i, \tilde{y}_i)$ of the $(k+\ell)$ -dimensional generalized eigenvalue problem $(AZ)^TAZ\tilde{y} = \tilde{\lambda}Z^TAZ\tilde{y}$. 17/37

DCG for multiple right-hand sides (DCGMRHS)

- Given a sequence $\{b^{(s)}\}_{s=1,...,\nu}$, solve for $\{x^{(s)}\}_{s=1,...,\nu}$ s.t. $Ax^{(s)}=b^{(s)}$:

 1/Solve for $x^{(1)} \in \mathcal{K}_*(A, r_0^{(1)})$ by CG. Store basis $V_\ell^{(1)}$ of $\mathcal{K}_\ell(A, r_0^{(1)})$.
 - 2/Get eigenpair approximations $\{(\tilde{\lambda}_i^{(1)}, w_i^{(1)})\}_{i=1,...,k}$ of A:

$$w_i^{(1)} \in A\mathcal{K}_{\ell}(A, r_0^{(1)})$$
 Solve $G^{(1)}\tilde{y}_i = \tilde{\lambda}_i^{(1)}F^{(1)}\tilde{y}_i$ with $G^{(1)} := (AV_{\ell}^{(1)})^TAV_{\ell}^{(1)}$
$$w_i^{(1)} := AV_{\ell}^{(1)}\tilde{y}_i$$

$$F^{(1)} := V_{\ell}^{(1)}AV_{\ell}^{(1)}$$

- **3.1/**Solve for $x^{(s)} \in \mathcal{K}_{k,*}(A, W^{(s-1)}, r_0^{(s)})$ by DCG. Store basis $V_{\ell}^{(s)}$ of $\mathcal{K}_{\ell}(A, r_0^{(s)})$. Let $Z^{(s)} := [W^{(s-1)}, V_{\ell}^{(s)}]$.
- 3.2/Get approximations $\{(\tilde{\lambda}_i^{(s)}, w_i^{(s)})\}_{i=1,...,k}$:

$$w_i^{(s)} \in A\mathcal{K}_{k,\ell}(A, W^{(s-1)}, r_0^{(s)})$$
 with $G^{(s)}$

$$A^{-1}w_i^{(s)} - w_i^{(s)}/\tilde{\lambda}_i^{(s)} \perp A\mathcal{K}_{k,\ell}(A, W^{(s-1)}, r_0^{(s)})$$

$$w_i^{(s)} := AZ_\ell^{(s)} \tilde{y}_i$$

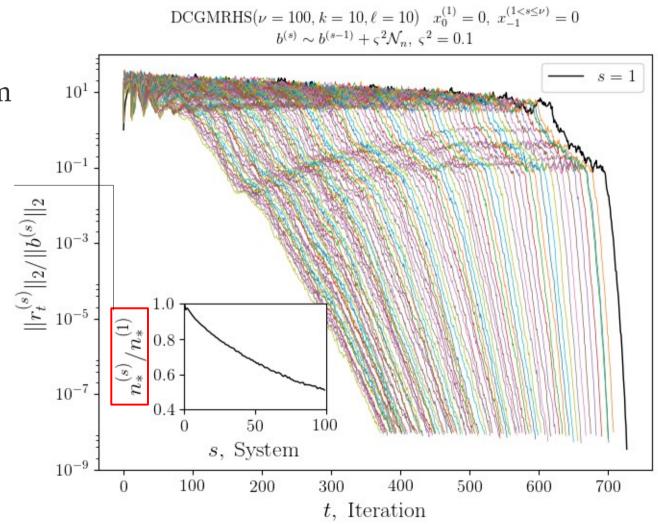
Solve
$$G^{(s)}\tilde{y}_{i} = \tilde{\lambda}_{i}^{(s)}F^{(s)}\tilde{y}_{i}$$

with $G^{(s)} := (AZ_{\ell}^{(s)})^{T}AZ_{\ell}^{(s)}$
 $F^{(s)} := Z_{\ell}^{(s)}^{T}AZ_{\ell}^{(s)}$
 $\vdots = AZ_{\ell}^{(s)}\tilde{x}_{\ell}$

- Let A be a single, fixed realization of the operator with $(\sigma^2, \ell) = (0.2, 0.1)$ $b^{(1)} \sim \mathcal{N}(0, I_n)$ and $b^{(s+1)} \sim b^{(s)} + \varsigma \mathcal{N}(0, I_n)$ for $1 \le s < \nu = 100$ with $\varsigma^2 = 0.1$
- Each curve stands for the evolution of the relative iterated residual of a system $Ax^{(s)} = b^{(s)}$.
- Relative gain of iterations for the s-th system wrt the 1st system to reach the stopping criterion:

$$\frac{\|r_t^{(s)}\|_2}{\|b^{(s)}\|_2} \le 10^{-8}$$

• $(k, \ell) = (10, 10)$

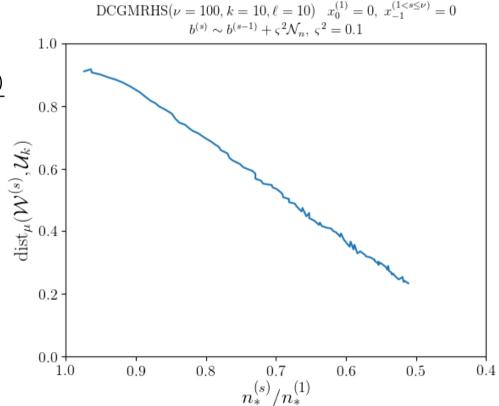


DCGMRHS – Effect of quality of eigenvectors approximation

- Deflation is performed with subspaces $\mathcal{W}^{(s)}$ spanned by approximations $\{w_i^{(s)}\}_{i=1}^k$ of the eigenvectors $\{u_i\}_{i=1}^k$ associated with the least dominant eigenvalues $\lambda_1 \leq \cdots \leq \lambda_k$ of A.
- The quality of this approximation can be measured by the principal angles $\{\theta_i^{(s)}\}_{i=1}^k$ between $\mathcal{W}^{(s)}$ and

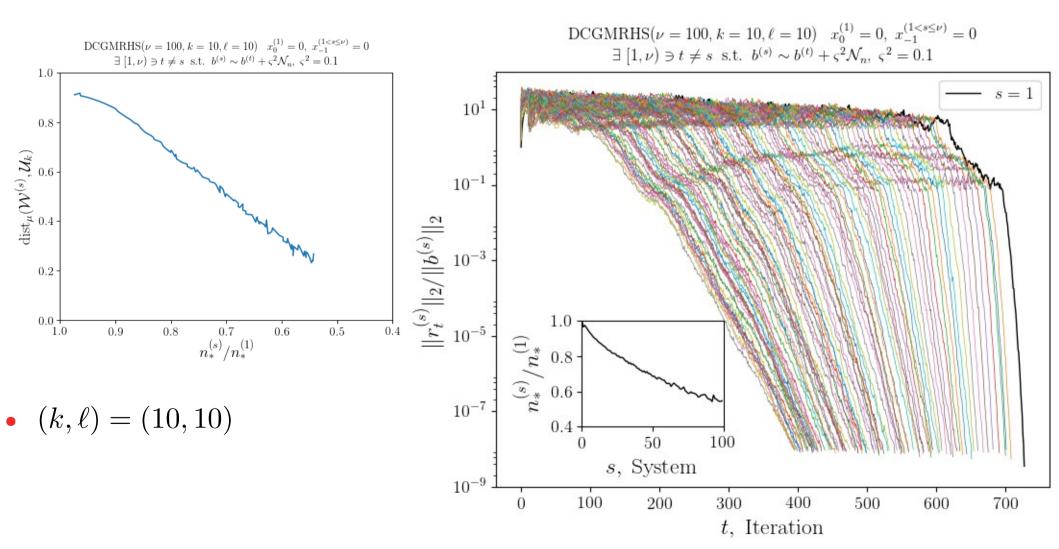
 $\mathcal{U}_k := \operatorname{span}\{u_1, \dots, u_k\}$.

• Let $\operatorname{dist}_{\mu}(\mathcal{W}^{(s)}, \mathcal{U}_k) := \sum_{i=1}^k \frac{\sin(\theta_i^{(s)})}{k}$

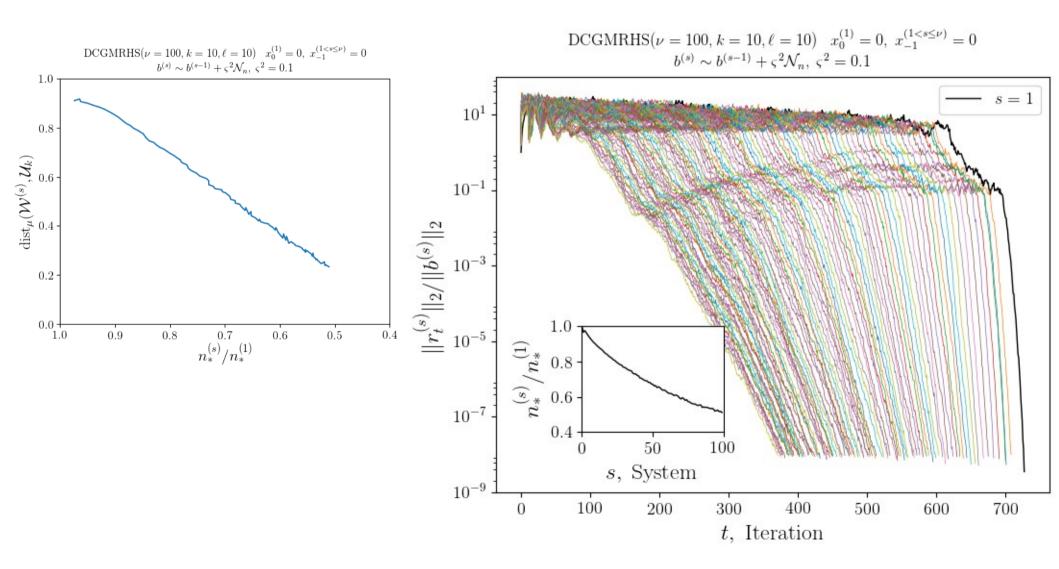


DCGMRHS results - Shuffled walk

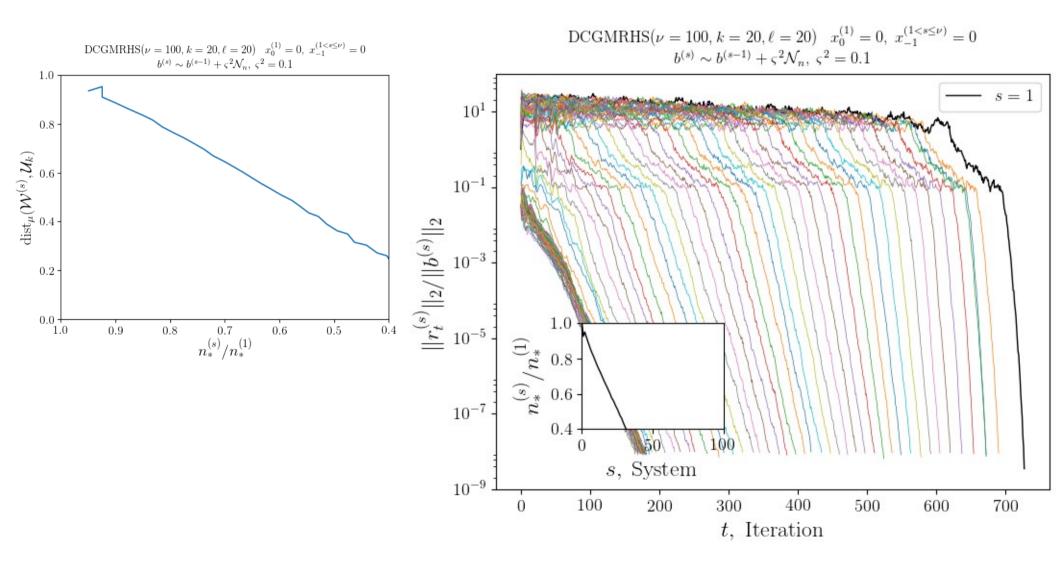
• Let A be the same realization as before. Let $\{b^{(s)}\}_{s=1}^{\nu}$ be the same samples as before, but randomly shuffled.



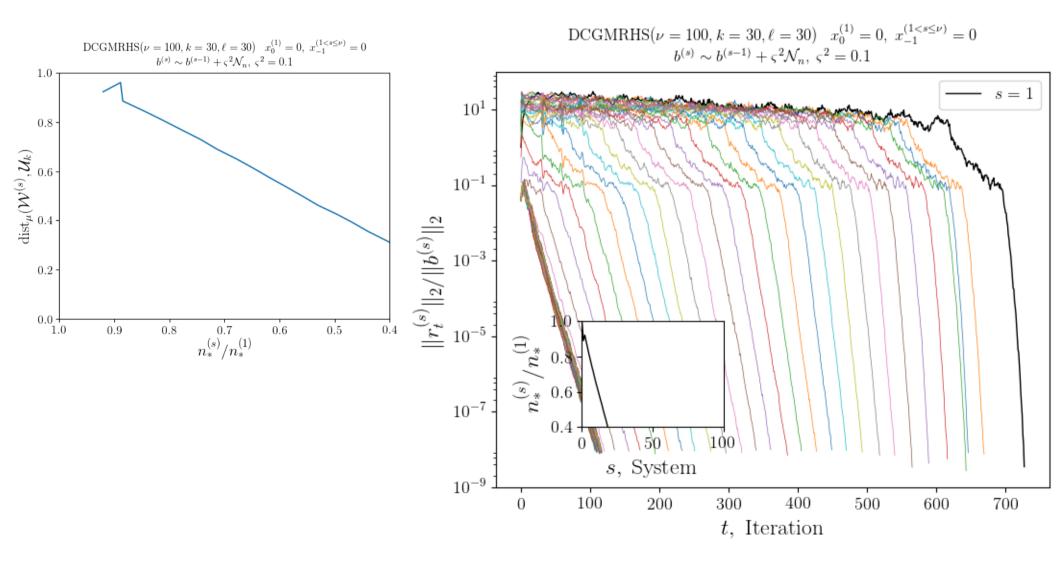
• Let's increase $(k, \ell) = (10, 10)$



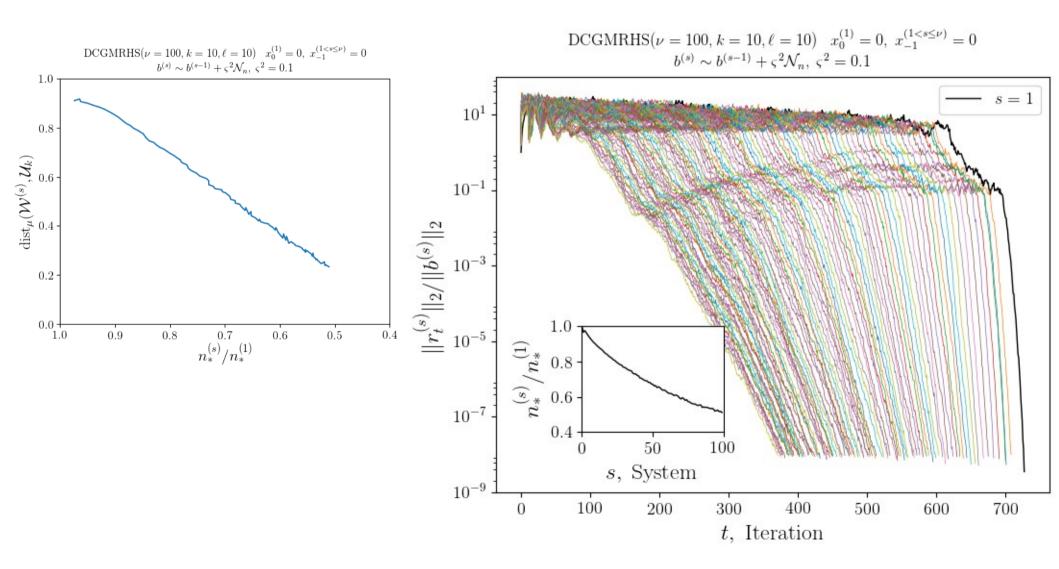
to
$$(k, \ell) = (20, 20)$$



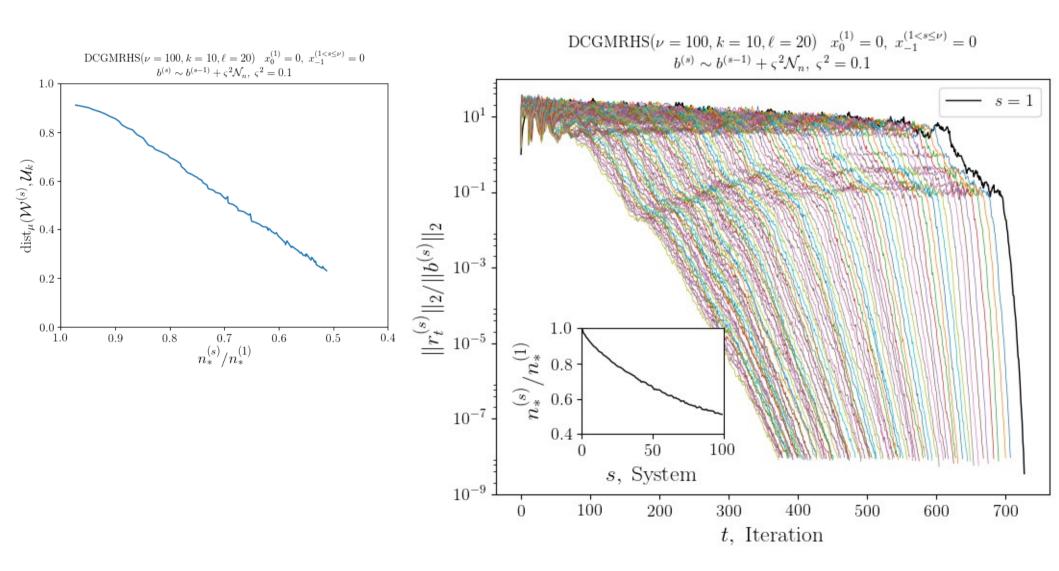
to
$$(k, \ell) = (30, 30)$$



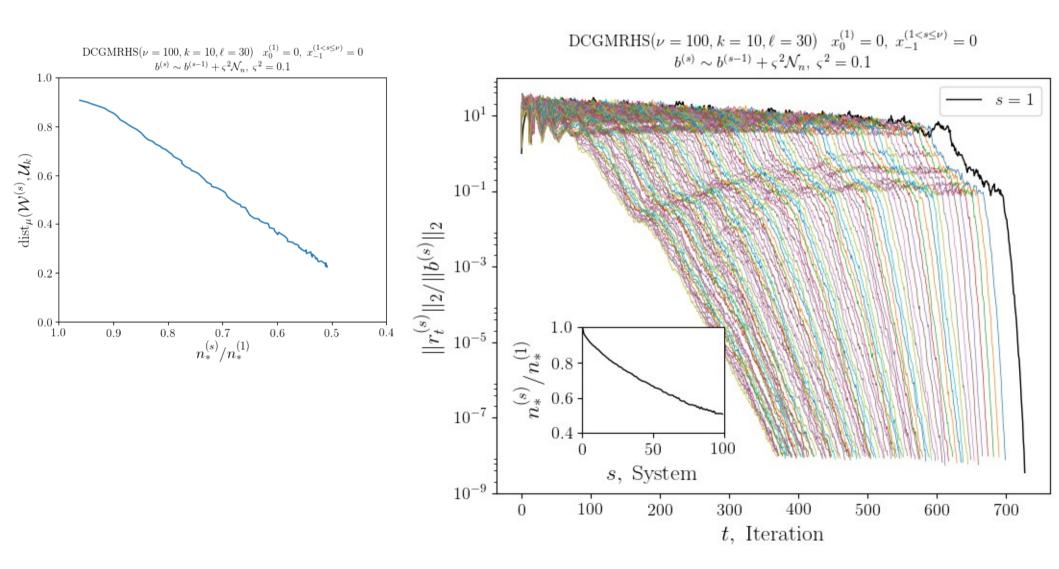
• Let's increase $(k, \ell) = (10, 10)$



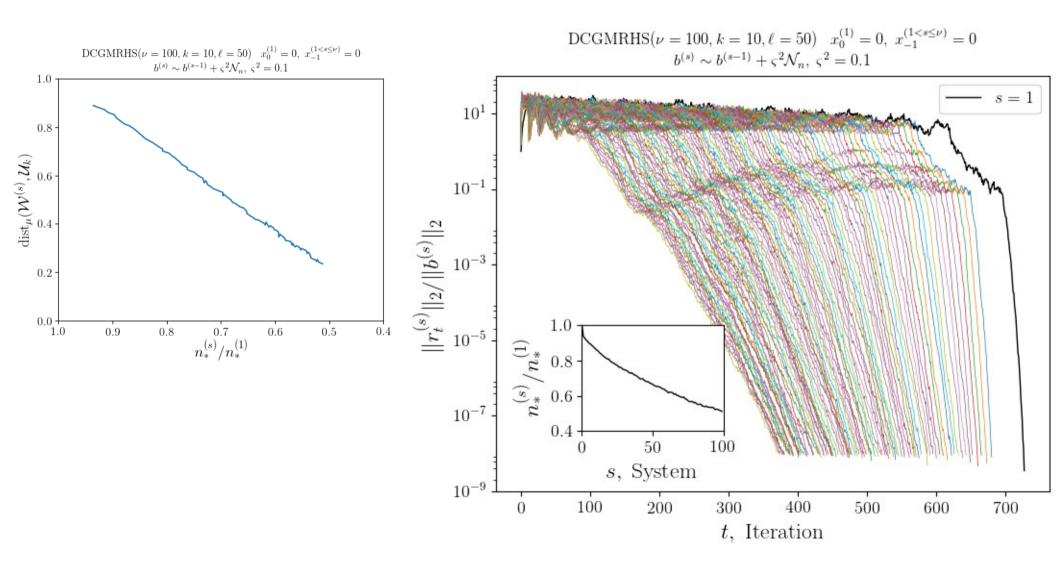
to
$$(k, \ell) = (10, 20)$$



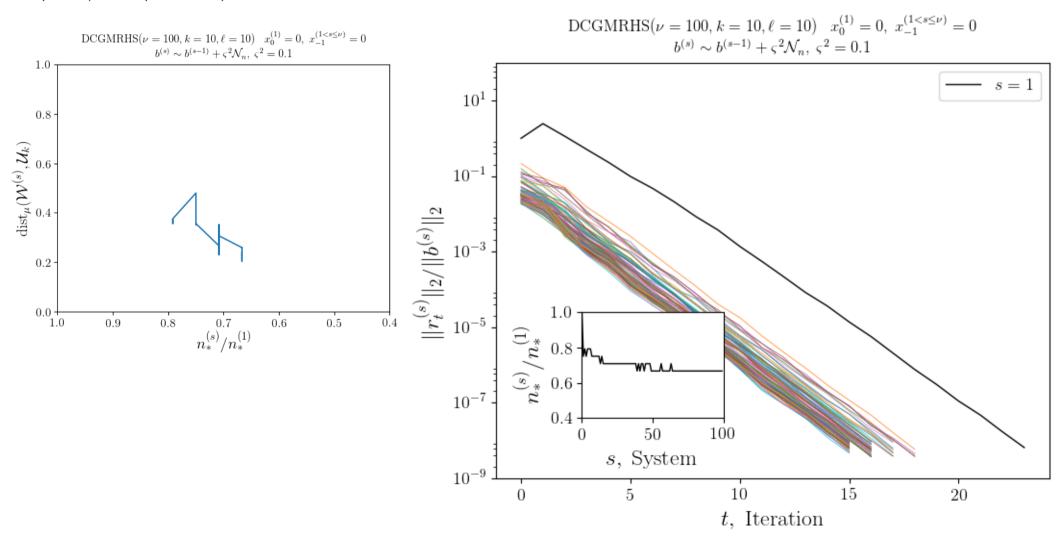
to
$$(k, \ell) = (10, 30)$$



to
$$(k, \ell) = (10, 50)$$



- Let's apply the preconditioner $M = A(\xi_1 = 0, ..., \xi_{n_{\rm KL}=0})$
- $(k, \ell) = (10, 10)$



DCG for multiple operators (DCGMO)

- Given a sequence $\{A^{(s)}\}_{s=1,...,\nu}$ solve for $\{x^{(s)}\}_{s=1,...,\nu}$ s.t. $A^{(s)}x^{(s)}=b$:
 - **1/**Solve for $x^{(1)} \in \mathcal{K}_*(A^{(1)}, r_0^{(1)})$ by CG. Store basis $V_\ell^{(1)}$ of $\mathcal{K}_\ell(A^{(1)}, r_0^{(1)})$.
 - 2/Get eigenpair approximations $\{(\tilde{\lambda}_i^{(1)}, w_i^{(1)})\}_{i=1,\dots,k}$ of $A^{(1)}$:

- **3.1/**Solve for $x^{(s)} \in \mathcal{K}_{k,*}(A^{(s)}, W^{(s-1)}, r_0^{(s)})$ by DCG. Store basis $V_{\ell}^{(s)}$ of
- $\mathcal{K}_{\ell}(A^{(s)}, r_0^{(s)})$. Let $Z^{(s)} := [W^{(s-1)}, V_{\ell}^{(s)}]$.
- 3.2/Get approximations $\{(\tilde{\lambda}_i^{(s)}, w_i^{(s)})\}_{i=1,...,k}$ of eigenpairs of $A^{(s)}$:

$$w_{i}^{(s)} \in A^{(s)} \mathcal{K}_{k,\ell}(A^{(s)}, W^{(s-1)}, r_{0}^{(s)})$$

$$A^{(s)^{-1}} w_{i}^{(s)} - w_{i}^{(s)} / \tilde{\lambda}_{i}^{(s)} \perp A^{(s)} \mathcal{K}_{k,\ell}(A^{(s)}, W^{(s-1)}, r_{0}^{(s)})$$

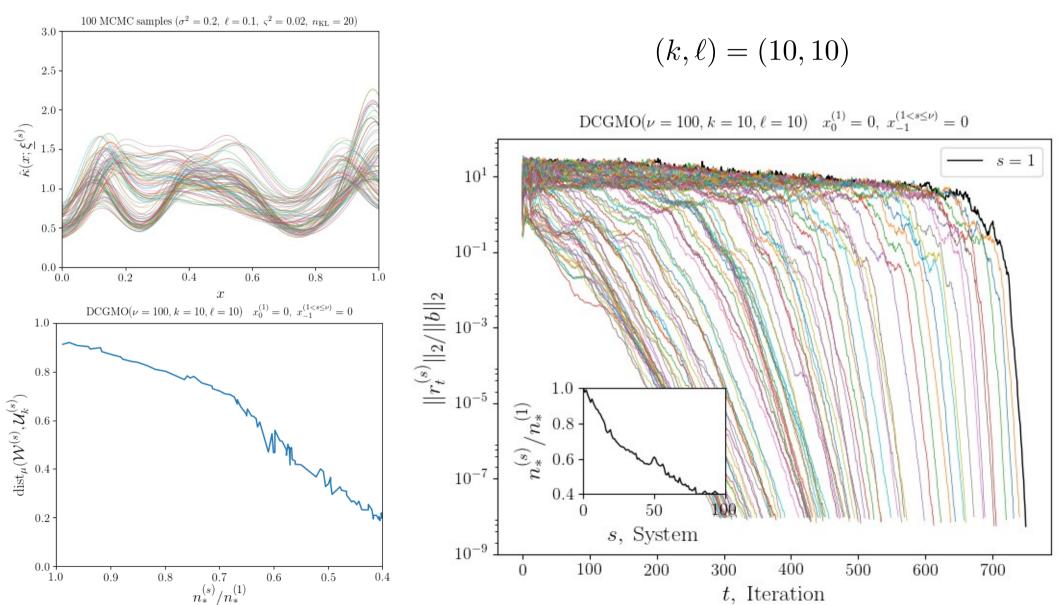
$$w_{i}^{(s)} := Z_{\ell}^{(s)^{T}} A^{(s)} Z_{\ell}^{(s)} \tilde{y}_{i}$$

$$w_{i}^{(s)} := A^{(s)} Z_{\ell}^{(s)} \tilde{y}_{i}$$

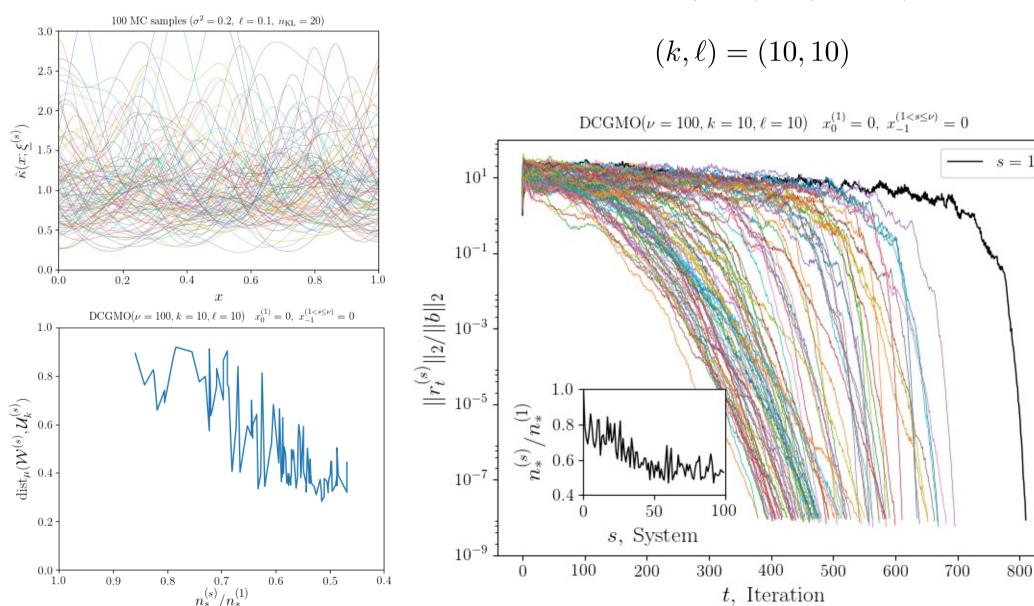
Solve $G^{(s)}\tilde{y}_i = \tilde{\lambda}_i^{(s)}F^{(s)}\tilde{y}_i$ with $G^{(s)} := (A^{(s)} Z_{\ell}^{(s)})^T A^{(s)} Z_{\ell}^{(s)}$ $F^{(s)} := Z_{\ell}^{(s)}{}^{T} A^{(s)} Z_{\ell}^{(s)}$

$$F^{(s)} := Z_{\ell}^{(s)} A^{(s)} Z_{\ell}^{(s)}$$
 $M^{(s)} := A^{(s)} Z^{(s)} \tilde{q}_{\ell}$

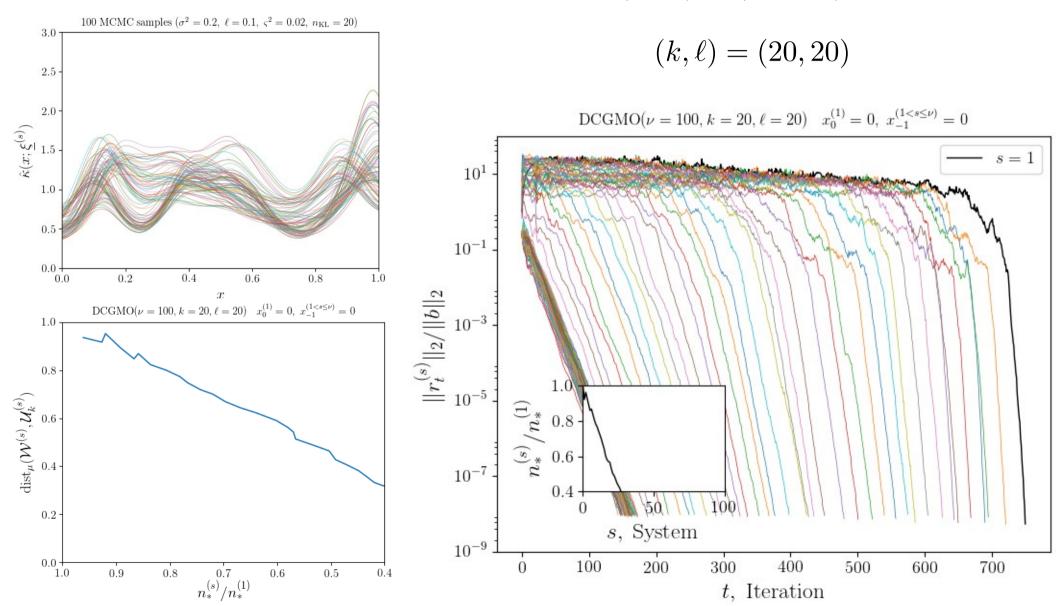
• Let $\{A^{(s)}\}_{s=1}^{100}$ be sampled by MCMC with $(\sigma^2, \ell) = (0.2, 0.1)$ and $\varsigma^2 = 0.02$



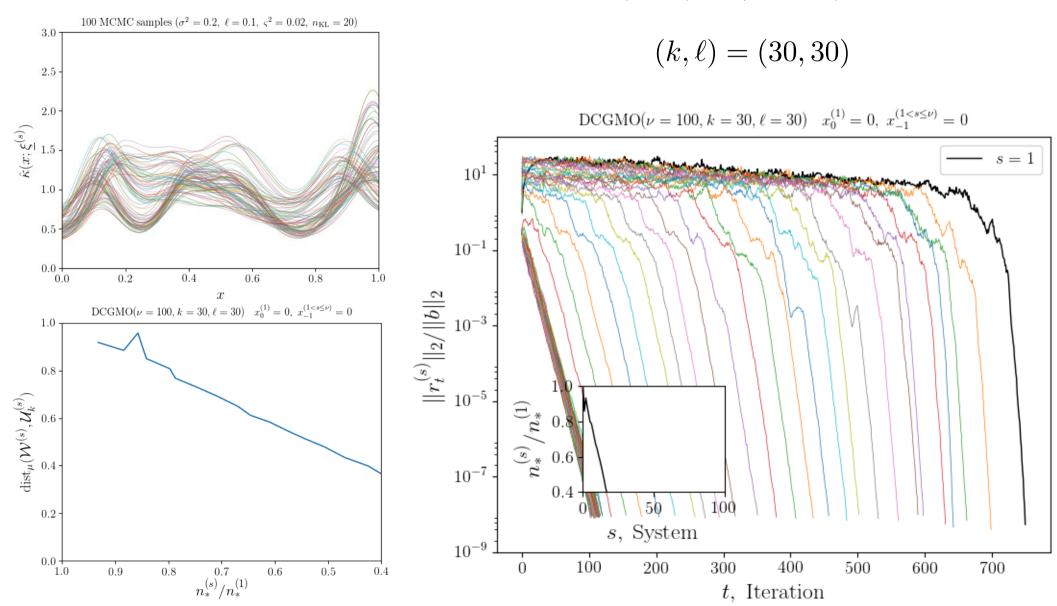
• Let $\{A^{(s)}\}_{s=1}^{100}$ be sampled by regular MC with $(\sigma^2,\ell)=(0.2,0.1)$.



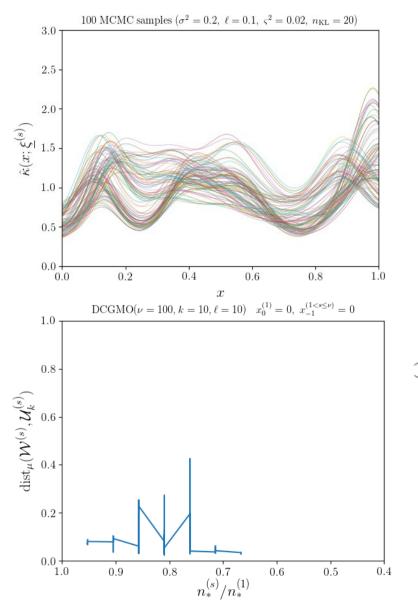
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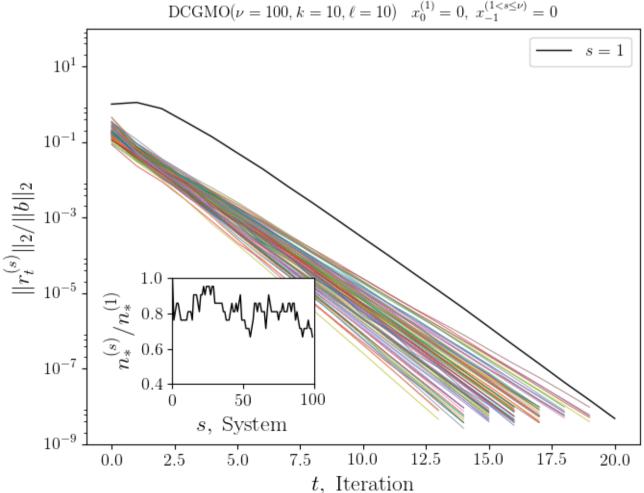
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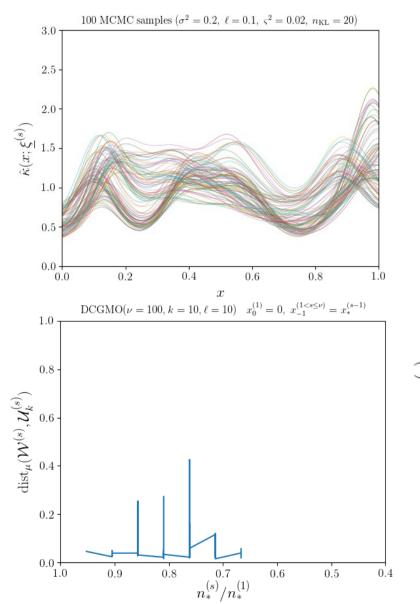
• Let $\{A^{(s)}\}_{s=1}^{100}$ be sampled by MCMC with $(\sigma^2, \ell) = (0.2, 0.1)$ and $\varsigma^2 = 0.02$



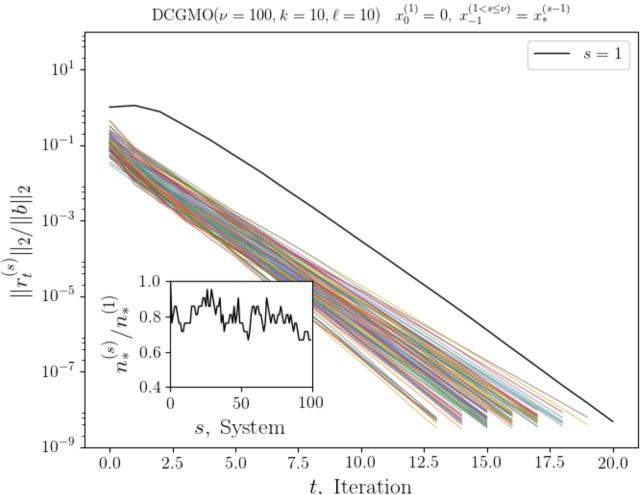
$(k, \ell) = (10, 10)$ with preconditioner



• Let $\{A^{(s)}\}_{s=1}^{100}$ be sampled by MCMC with $(\sigma^2, \ell) = (0.2, 0.1)$ and $\varsigma^2 = 0.02$



$$(k, \ell) = (10, 10)$$
 with preconditioner



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