

funNystrom 2

or

Algorithm-agnostic low-rank approximation of
operator monotone matrix functions

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Motivation

Given time series data, fit Gaussian Process to data with kernel function $K(\underline{x}, \underline{x}')$ and noise of variance σ

$$A = K + \sigma^2 I \quad , \quad [K]_{ij} = K(\underline{x}_i, \underline{x}_j)$$

To learn σ , maximize log-likelihood

$$\log \Pr[\underline{y} | \underline{x}_1, \dots, \underline{x}_n, \sigma] = \underbrace{\hspace{10em}} + \frac{1}{2} \underbrace{\log \det(K + \sigma^2 I)}_{\text{Need to compute this}}$$

How to compute $\log \det(K + \sigma^2 I)$?

$$\log \det(K + \sigma^2 I) = \text{tr}(\log(A))$$

Naïve Algo:

- ① Use Lanczos to approx $\underline{x} \rightarrow \log(A)\underline{x}$
- ② Run Hutch++

Lanczos is slow. Can we do better?

Hutch++

- ① Find $B \approx (\log(A))_K$
- ② Compute $\underline{x}^T (\log(A) - B) \underline{x}$ many times

We focus on ①

$f(A)$ **Low-Rank Approximation**

Given $\overset{\text{PSD}}{A} \in \mathbb{R}^{n \times n}$, K , $\varepsilon > 0$, $f: \mathbb{R} \rightarrow \mathbb{R}$ find matrix $C \in \mathbb{R}^{n \times K}$ with

$$\|f(A) - C\|_{F,2} \leq (1 + \varepsilon) \|f(A) - (f(A))_K\|_{F,2}$$

Naively: Lanczos to approximate $f(A)_{\underline{x}}$, run Krylov

Ideally, what should C be?

Low-Rank Approx and Matrix Functions

Eigendecomposition $A = U \Lambda U^T$

$$\boxed{A} = \boxed{U} \boxed{\begin{array}{c} \lambda_1 \\ \vdots \\ \lambda_n \end{array}} \boxed{U^T}$$

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0$$

Best rank- k approx $= A_k$ = zero out all except k largest eigs

Matrix Function $= f(A) = U f(\Lambda) U^T$

$$\boxed{A} = \boxed{U} \boxed{\begin{array}{c} f(\lambda_1) \\ \vdots \\ f(\lambda_k) \end{array}} \boxed{U^T}$$

Best rank- k approx $= (f(A))_k$ = zero all except k largest of $f(A)$

$$f(x) \geq 0, \text{ } f \text{ increasing} \\ f(0) = 0$$

= zero all except k largest of A

$$= f(A_k)$$

$f(A_k)$ takes $O(n^2 k)$ time to compute!

Meta-algo

(our result, informally:
this is always a good idea)

Since $(f(A))_K = f(A_K)$

① Find low-rank $B \approx A_K$

② Compute $C = f(B)$

$O(n^2 K)$ time

③ Return C_K

allows $f(0) \neq 0, \text{rank}(B) > K$

Avoids Lanczos! $C_K \approx (f(A))_K$ Without accessing $f(A)$!

Problem: B must be symmetric PSD for $f(B)$ to exist

funNystrom [Persson Kresner]

Nystrom Approximation

Given ortho $Q \in \mathbb{R}^{n \times k}$, let $B = A Q (Q^T A Q)^{-1} Q^T A$

Then,

B is the best rank- k PSD approx to A in $\text{range}(AQ)$

- ① Run subspace iteration to find good Q
- ② Build $B = A Q (Q^T A Q)^{-1} Q^T A$
- ③ Return $(f(B))_k$

Thm: If f is "nice" then $O\left(\frac{n^2}{g_{k \rightarrow k+1}} \log \frac{1}{\epsilon}\right)$ time suffices

$$\uparrow \text{Eigengap} = \frac{\lambda_{k+1} - \lambda_k}{\lambda_{k+1}}$$

funNystrom Proof Sketch

f is **Operator Monotone** if

- for $A \preceq B$ we have $f(A) \preceq f(B)$
- implies f is concave (unintuitive)

Proof Sketch

- ① f is concave, so eigengaps of $f(A)$ are \leq those of A
- ② Subspace iter convergest fast when eigengaps large
- ③ A would need $O(\frac{1}{g_{K \rightarrow K+1}} \log(\frac{1}{\epsilon}))$ steps of subspace iter
- ④ A needs $O(\frac{1}{g_{K \rightarrow K+1}} \log(\frac{1}{\epsilon}))$ steps for funNystrom to converge
 $= O(\frac{n^2}{g_{K \rightarrow K+1}} \log(\frac{1}{\epsilon}))$ time

Our Contribution

Their proof is specific to subspace iteration

We often use other algos (Krylov, ID, Sketching, ...)

Thms

Let ortho $Q \in \mathbb{R}^{n \times K+p}$ s.t. $\|A - (QQ^T A)_K\|_{F,2,*} \leq (1+\epsilon) \|A - A_K\|_{F,2,*}$

Then $B = (A Q (Q^T A Q)^{-1} Q^T A)_K$ has $\|A - B\|_{F,2,*} \leq (1+\epsilon) \|A - A_K\|_{F,2,*}$

And $C = (f(B))_K$ has $\|f(A) - C\|_{F,2,*} \leq (1+\epsilon) \|f(A) - (f(A))_K\|_{F,2,*}$

Key points: algorithm agnostic, same value of ϵ !

(some nuances hidden, see paper)

Takeaways

If *Algo* produces ε -good Q in time τ ,
then funNystrom is ε -good in time $\tau + O(n^\tau \kappa)$

Proofs: boring & short

Ready for implementation!

Secondary motivation:

If $f(A)$ has quickly decaying eigenvalues,

Then funNystrom(A) preserves "all" structure of $f(A)$ fast!

Future Directions: Beyond operator monotone (log-concave?)