Fast Low-Rank Factorization of Kernel Matrices through Skeletonized Interpolation

Leopold Cambier*, Eric Darve
*lcambier@stanford.edu
Institute of Computational and Mathematical Engineering

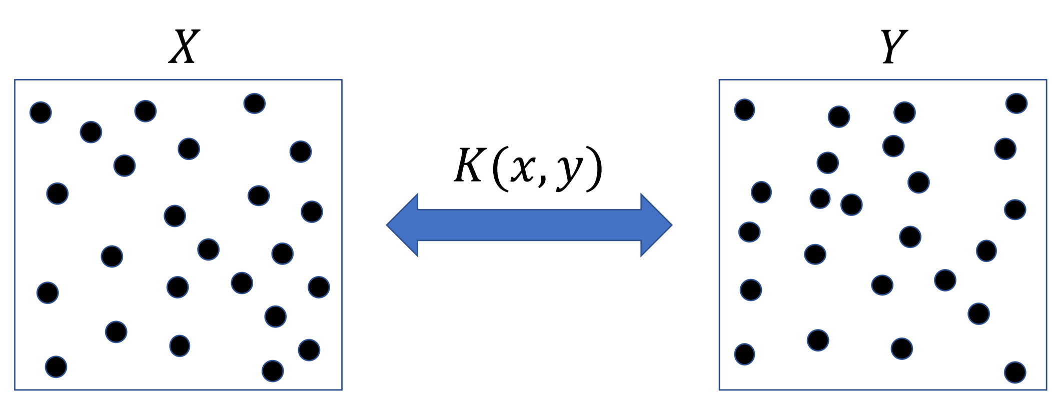
Overview

Given $X = \{x_1, \dots, x_n\}$, $Y = \{y_1, \dots, y_n\}$ and $K(x,y)$ smooth, build low-rank factorization of

$$K_{ij} = K(x_i, y_j)$$

The resulting algorithm

- has near-optimal complexity $\mathcal{O}(nr)$ with small constants, where r is the optimal rank
- is insensible to points X and Y distribution
- is very easy to implement
- is numerically very stable and accurate
- can work in arbitrary spaces using a smooth mapping



Motivation

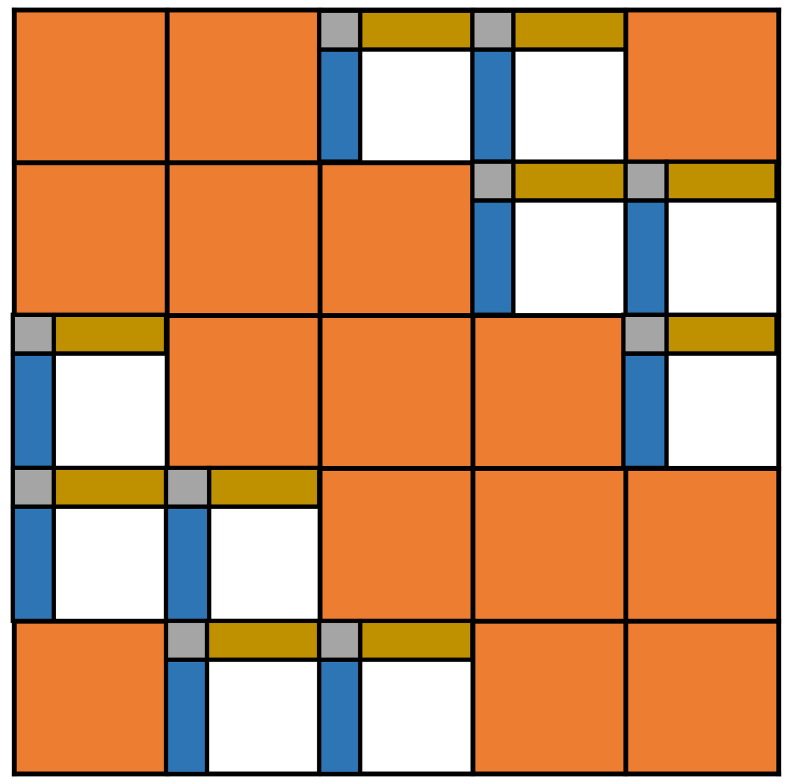
Many physical problems can be modeled as *integral equations*

$$a(x)u(x) + \int_{\partial\Omega} K(x,y)u(y)\mathrm{d}y = f(x) \quad \forall x \in \partial\Omega$$

that, after discretization, give

$$a_i u_i + \sum_{k=1}^{N} K_{ij} u_j = f_i \quad \forall i.$$

In that case, K's off-diagonal blocks are low-rank



Continuous SVD

If K is smooth there exists a continuous SVD,

$$K(x,y) = \sum_{s=1}^{\infty} \sigma_s u_s(x) v_s(y)$$
$$\approx \sum_{s=1}^{r} \sigma_s u_s(x) v_s(y)$$

Given this, one has

$$K(X,Y) \approx \begin{bmatrix} | & & | \\ u_1(X) & \dots & u_r(X) \\ | & & | \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{bmatrix} \begin{bmatrix} | & & | \\ v_1(Y) & \dots & v_r(Y) \\ | & & | \end{bmatrix}^\top$$

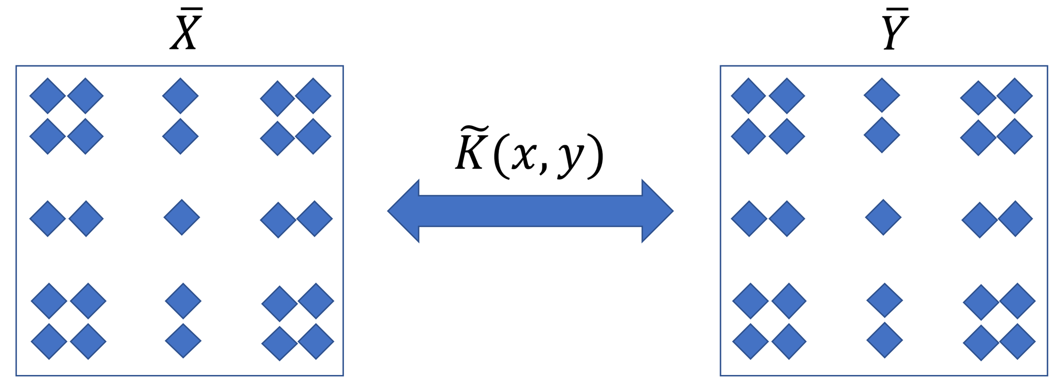
Problem becomes: find a low-rank approximation of $K(x,y)$, since then $K(X,Y)$ follows.

Kernel Interpolation

By interpolating in x and y successively,

$$K(x,y) \approx \sum_{k=1}^{K} L_k(x) K(\bar{x}_k, y)$$
$$\approx \sum_{k=1}^{K} \sum_{l=1}^{L} L_k(x) K(\bar{x}_k, \bar{y}_l) L_l(y)$$
$$= \tilde{K}(x,y)$$

using tensor of Chebyshev nodes $\bar{x}_k$ and $\bar{y}_l$ over X and Y.



So

$$K(X,Y) \approx \tilde{K}(X,Y) =$$
$$\begin{bmatrix} | & & | \\ L_1(X) & \dots & L_K(X) \\ | & & | \end{bmatrix} \begin{bmatrix} K(\bar{x}_1, \bar{y}_1) & \dots & K(\bar{x}_1, \bar{y}_L) \\ \vdots & & \vdots \\ K(\bar{x}_K, \bar{y}_1) & \dots & K(\bar{x}_K, \bar{y}_L) \end{bmatrix} \begin{bmatrix} | & & | \\ L_1(Y) & \dots & L_L(Y) \\ | & & | \end{bmatrix}^\top$$

Issue

Rank of $\tilde{K}$, r_0, is usually much higher than r.

Skeletonized Interpolation

- $K(\bar{X}, \bar{Y})$ has rank $r_0 \gg r$
- Need to recompress
- CUR decomposition selects $\hat{X} \subset \bar{X}$ and $\hat{Y} \subset \bar{Y}$ such that

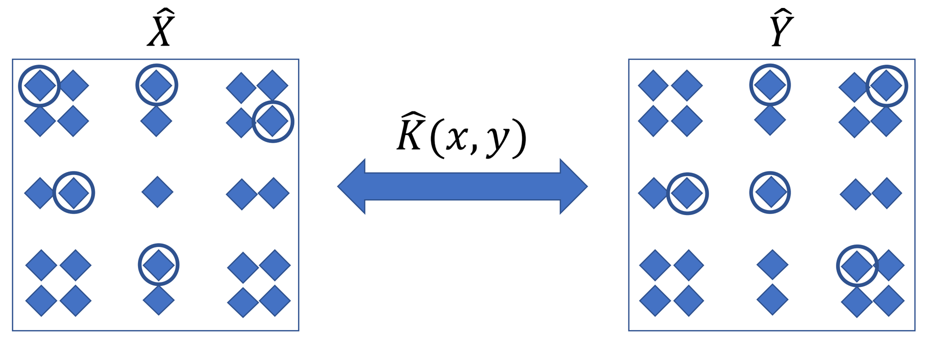
$$P_x K(\bar{X}, \bar{Y}) P_y \approx \begin{bmatrix} I \\ \check{S} \end{bmatrix} K(\hat{X}, \hat{Y}) \begin{bmatrix} I & \check{T}^\top \end{bmatrix}$$

where $\|\check{S}\|$, $\|\check{T}\|$ are small (in practice, one has to take into account the integration weights of the Chebyshev nodes as well)
- The obtained factorization is

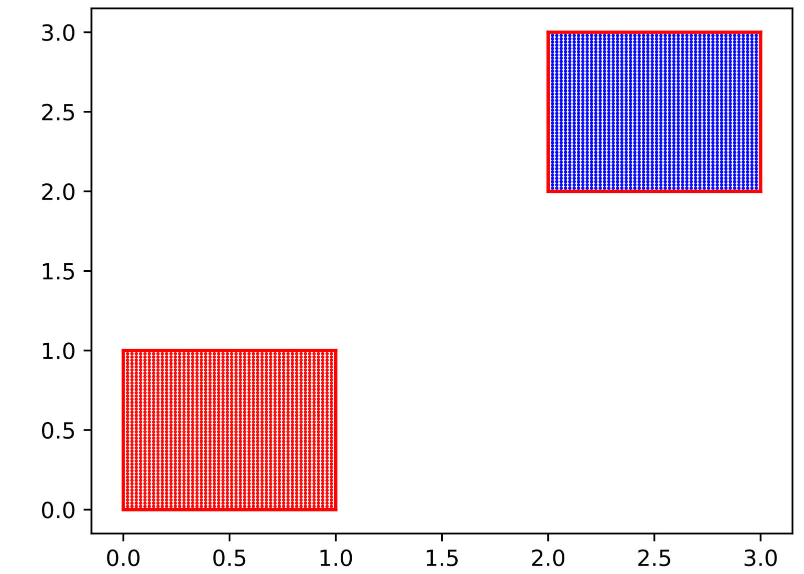
Skeletonized Interpolation

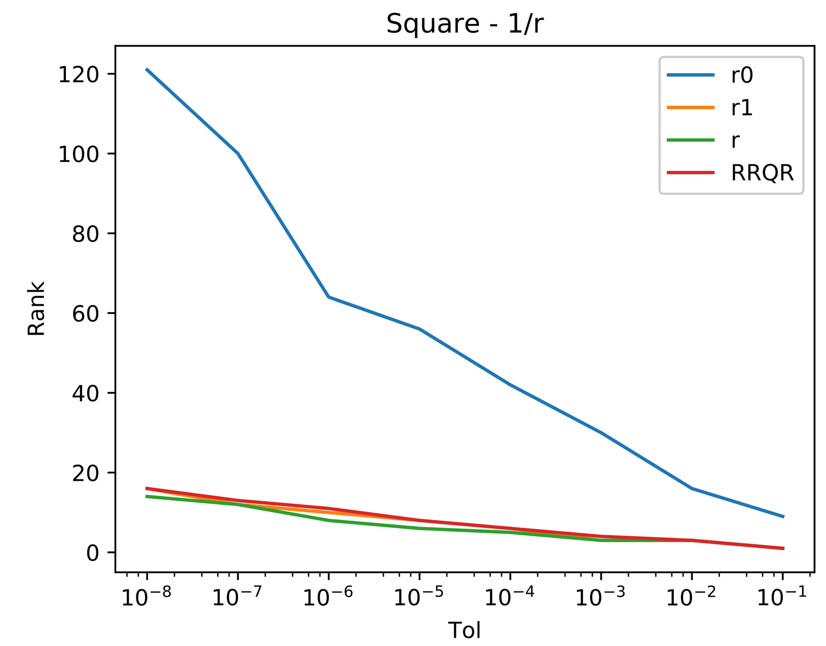
$$K(x,y) \approx \hat{K}(x,y) = K(x,\hat{Y}) K(\hat{X},\hat{Y})^{-1} K(\hat{X},y),$$

with rank $r_1 = |\hat{X}| = |\hat{Y}| \approx r$.



Numerical Results

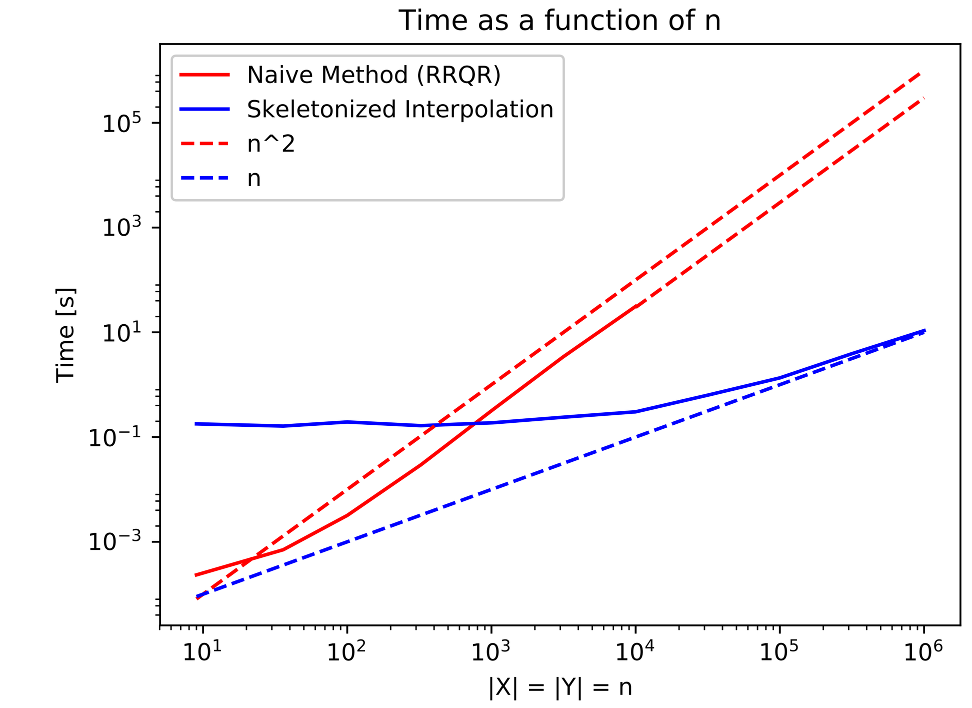


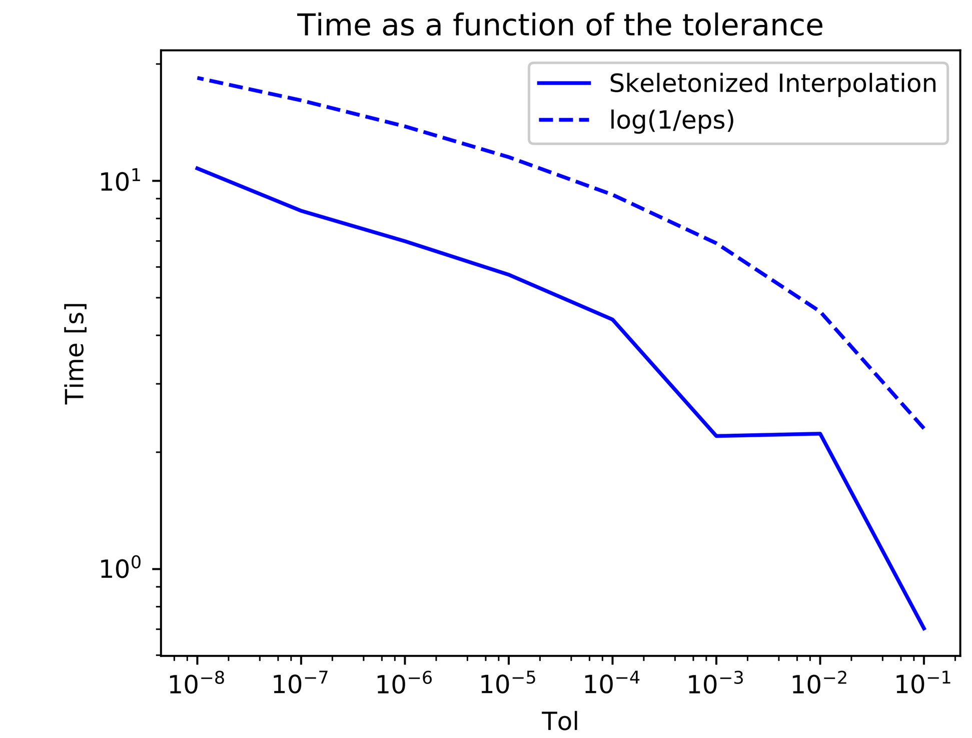


Computational Cost

Nearly optimal complexity of $\mathcal{O}(nr)$ to build the Skeletonized Interpolation factorization

$$K(X,Y) \approx K(X,\hat{Y}) K(\hat{X},\hat{Y})^{-1} K(\hat{X},Y).$$





Future Work

- Explore other interpolation rules
- Try sparse grids methods to work in higher dimensions

Bibliography

[1] L. Cambier, E. Darve. 'Fast Low-Rank Approximation of Kernel Matrices through Skeletonized Interpolation', 2017. In preparation.