



# Introduction to iterative methods

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Numerical Linear Algebra. Skoltech

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- If we want to solve partial eigenproblem, the full eigendecomposition is too costly.
- For both problems we will use iterative, Krylov subspace solvers, which treat the matrix as a **black-box** linear operator.

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- **This is the only information** we know about the matrix: the matrix-by-vector product (matvec)
- Can we solve linear systems using only matvecs?
- Of course, we can multiply by the columns of the identity matrix, and recover the full matrix, but it is not what we need.

## ~~Gradient Descent~~ Richardson iteration

# Richardson iteration

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$$x_{k+1} = x_k - \tau(Ax_k - f),$$

where  $\tau$  is the **iteration parameter**, which can be always chosen such that the method **converges**.

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$$\frac{dy}{dt} + Ay = f, \quad y(0) = y_0.$$

- Then  $y(t) \rightarrow A^{-1}f$  as  $t \rightarrow \infty$ , and the **Euler scheme** reads

$$\frac{y_{k+1} - y_k}{\tau} = -Ay_k + f.$$

which leads to the Richardson iteration

$$y_{k+1} = y_k - \tau(Ay_k - f)$$

## Gradient flow ODE

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where  $x_k \equiv x(t_k)$  and  $\alpha = t_{k+1} - t_k$  - is the grid step.

From here we get the expression for  $x_{k+1}$

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Open In Colab 

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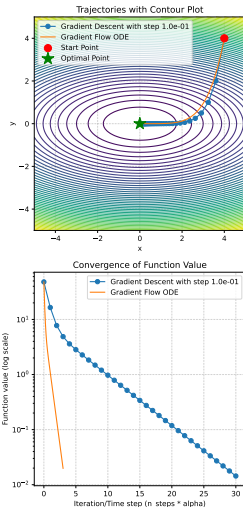


Figure 1: Gradient flow trajectory

# Convergence of the Richardson method

- Let  $x_*$  be the solution; introduce an error  $e_k = x_k - x_*$ , then

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- For symmetric positive definite case it is always possible to select  $\tau$  such that the method converges.
- What about the non-symmetric case? Below demo will be presented. . .



# Richardson method is equivalent to the Gradient Descent for quadratics

Consider the following quadratic optimization problem:

$$\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^d.$$

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- Let's show, that we can switch coordinates to make an analysis a little bit easier. Let  $\hat{x} = Q^T(x - x^*)$ , where  $x^*$  is the minimum point of initial function, defined by  $Ax^* = b$ . At the same time  $x = Q\hat{x} + x^*$ .



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$$\begin{aligned} f(\hat{x}) &= \frac{1}{2} (Q\hat{x} + x^*)^\top A (Q\hat{x} + x^*) - b^\top (Q\hat{x} + x^*) \\ &= \frac{1}{2} \hat{x}^\top Q^\top A Q \hat{x} + (x^*)^\top A Q \hat{x} + \frac{1}{2} (x^*)^\top A (x^*) - b^\top Q \hat{x} - b^\top x^* \end{aligned}$$



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# Convergence of the ~~Richardson method~~ Gradient Descent

Now we can work with the function  $f(x) = \frac{1}{2}x^T \Lambda x$  with  $x^* = 0$  without loss of generality (drop the hat from the  $\hat{x}$ )

$$x^{k+1} = x^k - \alpha \nabla f(x^k)$$



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Let's use constant stepsize  $\alpha^k = \alpha$ . Convergence condition:

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Remember, that  $\lambda_{\min} = \mu > 0, \lambda_{\max} = L \geq \mu$ .

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Now we would like to tune  $\alpha$  to choose the best (lowest) convergence rate

$$\rho^* = \min_{\alpha} \rho(\alpha)$$

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$$x^{k+1} = \left(\frac{L - \mu}{L + \mu}\right)^k x^0 \quad f(x^{k+1}) = \left(\frac{L - \mu}{L + \mu}\right)^{2k} f(x^0)$$

## Convergence analysis

So, we have a linear convergence in the domain with rate  $\frac{\kappa-1}{\kappa+1} = 1 - \frac{2}{\kappa+1}$ , where  $\kappa = \frac{L}{\mu}$  is sometimes called *condition number* of the quadratic problem.

$\kappa$	$\rho$	Iterations to decrease domain gap 10 times	Iterations to decrease function gap 10 times
1.1	0.05	1	1
2	0.33	3	2
5	0.67	6	3
10	0.82	12	6
50	0.96	58	29
100	0.98	116	58
500	0.996	576	288
1000	0.998	1152	576

## Optimal parameter choice

- The choice of  $\tau$  that minimizes  $\|I - \tau A\|_2$  for  $A = A^* > 0$  is (prove it!)

$$\tau_{\text{opt}} = \frac{2}{\lambda_{\min} + \lambda_{\max}}.$$

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- So, to find optimal parameter, we need to know the **bounds of the spectrum** of the matrix  $A$ , and we can compute it by using **power method**.

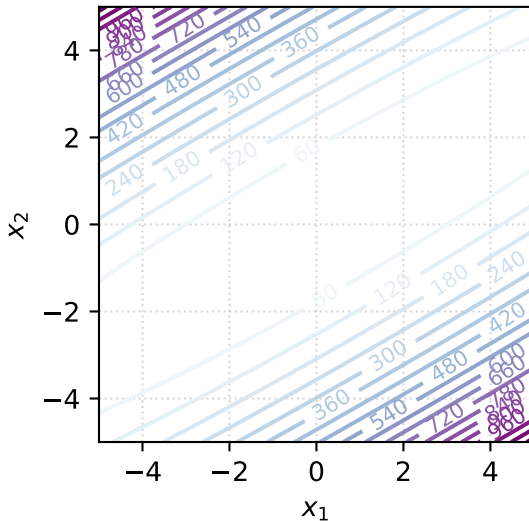


## Condition number

$\kappa = 1.5$



$\kappa = 50$



## Condition number and convergence speed

Even with the optimal parameter choice, the error at the next step satisfies

$$\|e_{k+1}\|_2 \leq q \|e_k\|_2, \quad \rightarrow \quad \|e_k\|_2 \leq q^k \|e_0\|_2,$$

where

$$q = \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} = \frac{\text{cond}(A) - 1}{\text{cond}(A) + 1},$$

$$\text{cond}(A) = \frac{\lambda_{\max}}{\lambda_{\min}} \quad \text{for } A = A^* > 0$$

is the condition number of  $A$ .

Let us do some demo...

# Demo



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Possible cases of Richardson iteration behaviour:

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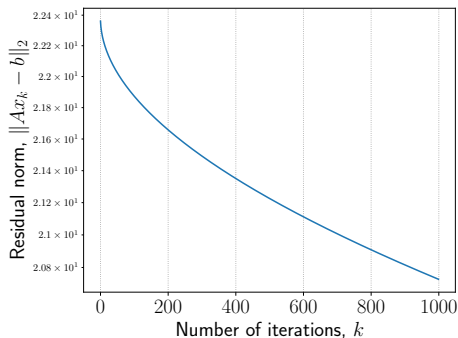
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Possible cases of Richardson iteration behaviour:

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**Q:** how can we identify our case **before** running iterative method?

## Spectrum directly affects the convergence



# One can still formulate a Lyapunov function <sup>1</sup>



<sup>1</sup>Another approach to build Lyapunov functions for the first order methods in the quadratic case. D. M. Merkulov, I. V. Oseledets

# Steepest Descent



# Better iterative methods

But before preconditioners, we can use **better iterative methods**.

There is a whole **zoo** of iterative methods, but we need to know just few of them.

## Attempt 1: The steepest descent method

- Suppose we **change**  $\tau$  every step, i.e.

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- This method is called **the steepest descent**.
- However, it still converges similarly to the Richardson iteration.

## Exact line search aka steepest descent

$$\alpha_k = \arg \min_{\alpha \in \mathbb{R}^+} f(x_{k+1}) = \arg \min_{\alpha \in \mathbb{R}^+} f(x_k - \alpha \nabla f(x_k))$$

More theoretical than practical approach. It also allows you to analyze the convergence, but often exact line search can be difficult if the function calculation takes too long or costs a lot. An interesting theoretical property of this method is that each following iteration is orthogonal to the previous one:

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Optimality conditions:

$$\nabla f(x_{k+1})^\top \nabla f(x_k) = 0$$



Figure 2: Steepest Descent

Open In Colab 

## Chebyshev iteration

## Attempt 2: Chebyshev iteration

Another way to find  $\tau_k$  is to consider

$$e_{k+1} = (I - \tau_k A)e_k = (I - \tau_k A)(I - \tau_{k-1} A)e_{k-1} = \dots = p(A)e_0,$$

where  $p(A)$  is a **matrix polynomial** (simplest matrix function)

$$p(A) = (I - \tau_k A) \dots (I - \tau_0 A),$$

and  $p(0) = 1$ .

# Optimal choice of time steps

The error is written as

$$e_{k+1} = p(A)e_0,$$

and hence

$$\|e_{k+1}\| \leq \|p(A)\| \|e_0\|,$$

where  $p(0) = 1$  and  $p(A)$  is a **matrix polynomial**.

To get better **error reduction**, we need to minimize

$$\|p(A)\|$$

over all possible polynomials  $p(x)$  of degree  $k + 1$  such that  $p(0) = 1$ . We will use  $\|\cdot\|_2$ .

# Polynomials least deviating from zeros

**Important special case:**  $A = A^* > 0$ .

Then,  $A = U\Lambda U^*$ ,

and

$$\|p(A)\|_2 = \|Up(\Lambda)U^*\|_2 = \|p(\Lambda)\|_2 = \max_i |p(\lambda_i)| \stackrel{!}{\leq} \max_{\lambda_{\min} \leq \lambda \leq \lambda_{\max}} |p(\lambda)|.$$

The latter inequality is the only approximation. Here we make a **crucial assumption** that we do not want to benefit from the distribution of the spectrum between  $\lambda_{\min}$  and  $\lambda_{\max}$ .

Thus, we need to find a polynomial  $p(\lambda)$  such that  $p(0) = 1$ , and which has the least possible deviation from 0 on  $[\lambda_{\min}, \lambda_{\max}]$ .

## Polynomials least deviating from zeros (2)

We can do the affine transformation of the interval  $[\lambda_{\min}, \lambda_{\max}]$  to the interval  $[-1, 1]$ :

$$\xi = \frac{\lambda_{\max} + \lambda_{\min} - (\lambda_{\min} - \lambda_{\max})x}{2}, \quad x \in [-1, 1].$$

The problem is then reduced to the problem of finding the **polynomial least deviating from zero** on an interval  $[-1, 1]$ .

## Exact solution: Chebyshev polynomials

The exact solution to this problem is given by the famous **Chebyshev polynomials** of the form

$$T_n(x) = \cos(n \arccos x)$$

# What do you need to know about Chebyshev polynomials

1. This is a polynomial!

We can plot them. . .



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3.  $|T_n(x)| \leq 1$  on  $x \in [-1, 1]$ .

We can plot them...

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4. It has  $(n + 1)$  **alternation points**, where the maximal absolute value is achieved (this is the sufficient and necessary condition for the **optimality**) (Chebyshev alternance theorem, no proof here).
5. The **roots** are just

$$n \arccos x_k = \frac{\pi}{2} + \pi k, \quad \rightarrow \quad x_k = \cos \frac{\pi(2k + 1)}{2n}, \quad k = 0, \dots, n - 1$$

We can plot them...

# Demo

## Convergence of the Chebyshev-accelerated Richardson iteration

Note that  $p(x) = (1 - \tau_n x) \dots (1 - \tau_0 x)$ , hence roots of  $p(x)$  are  $1/\tau_i$  and that we additionally need to map back from  $[-1, 1]$  to  $[\lambda_{\min}, \lambda_{\max}]$ . This results into

$$\tau_i = \frac{2}{\lambda_{\max} + \lambda_{\min} - (\lambda_{\max} - \lambda_{\min})x_i}, \quad x_i = \cos \frac{\pi(2i+1)}{2n} \quad i = 0, \dots, n-1$$

The convergence (we only give the result without the proof) is now given by

$$e_{k+1} \leq Cq^k e_0, \quad q = \frac{\sqrt{\text{cond}(A)} - 1}{\sqrt{\text{cond}(A)} + 1},$$

which is better than in the Richardson iteration.

- Permutation of roots of Chebyshev polynomial has crucial effect on convergence

# Demo

- Permutation of roots of Chebyshev polynomial has crucial effect on convergence
- On the optimal permutation you can read in paper (V. Lebedev, S. Finogenov 1971) (ru, en)



# Beyond Chebyshev

- We have made an important assumption about the spectrum: it is contained within an interval over the real line (and we need to know the bounds)

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- We have made an important assumption about the spectrum: it is contained within an interval over the real line (and we need to know the bounds)
- If the spectrum is contained within **two intervals**, and we know the bounds, we can also put the optimization problem for the **optimal polynomial**.

# Spectrum of the matrix contained in multiple segments

- For the case of **two segments** the best polynomial is given by **Zolotarev polynomials** (expressed in terms of elliptic functions). Original paper was published in 1877, see details [here](#)

# Spectrum of the matrix contained in multiple segments

- For the case of **two segments** the best polynomial is given by **Zolotarev polynomials** (expressed in terms of elliptic functions). Original paper was published in 1877, see details [here](#)
- For the case of **more than two segments** the best polynomial can be expressed in terms of **hyperelliptic functions**

## How can we make it better

- The implementation of the Chebyshev acceleration requires the knowledge of the spectrum.

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- It belongs to the class of **two-term** iterative methods, i.e. it approximates  $x_{k+1}$  using 2 vectors:  $x_k$  and  $r_k$ .
- It appears that if we **store more vectors**, then we can go without the spectrum estimation (and better convergence in practice)!



## Crucial point: Krylov subspace

The Chebyshev method produces the approximation of the form

$$x_{k+1} = x_0 + p(A)r_0,$$

i.e. it lies in the **Krylov subspace** of the matrix which is defined as

$$\mathcal{K}_k(A, r_0) = \text{Span}(r_0, Ar_0, A^2r_0, \dots, A^{k-1}r_0)$$

The most natural approach then is to find the vector in this **linear subspace** that minimizes certain **norm of the error**

# Idea of Krylov methods

The idea is to minimize given functional: - Energy norm of error for systems with hermitian positive-definite matrices (CG method). - Residual norm for systems with general matrices (MINRES and GMRES methods). - Rayleigh quotient for eigenvalue problems (Lanczos method).

To make methods practical one has to 1. Orthogonalize vectors  $A^i r_0$  of the Krylov subspace for stability (Lanczos process). 2. Derive recurrent formulas to decrease complexity.

We will consider these methods in details on the next lecture.

# Take home message

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- Main idea of iterative methods
- Richardson iteration: hermitian and non-hermitian case
- Chebyshev acceleration
- Definition of Krylov subspace

## Source

- NLA lecture by prof. Ivan Oseledets