Math 4997-3

Lecture 9: Solvers, Conjugate gradient method, and BlazeIterative

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Reminder

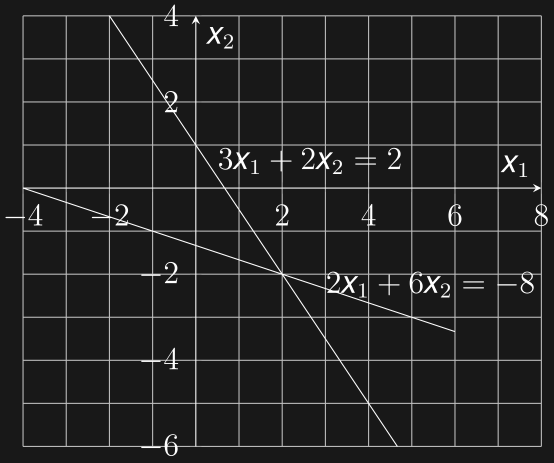
Lecture 9

What you should know from last lecture

- Vectors and matrices
- How to use Blaze for matrix and vector operations
- How to compile a program using a external library

Solving linear equation systems

Illustration of the linear system



Conjugate gradient method

Conjugate gradient method

Properties:

- Most popular iterative method for solving large systems of linear equations
- Developed by Hestenes and Stiefel in 1952 [3]
- Solves linear equation systems $\mathbf{A}\mathbf{x} = \mathbf{b}$
- Each iteration does one matrix-vector multiplication and some computation of inner products

Matrix

- Symmetry $\mathbf{A}^T = \mathbf{A}$
- Positive-definite $\mathbf{x}^T\mathbf{A}\mathbf{x} > 0, \forall \mathbf{x} > 0$

More details about iterative methods [2].

The quadratic form

Let us define the problem as a matrix:

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

with

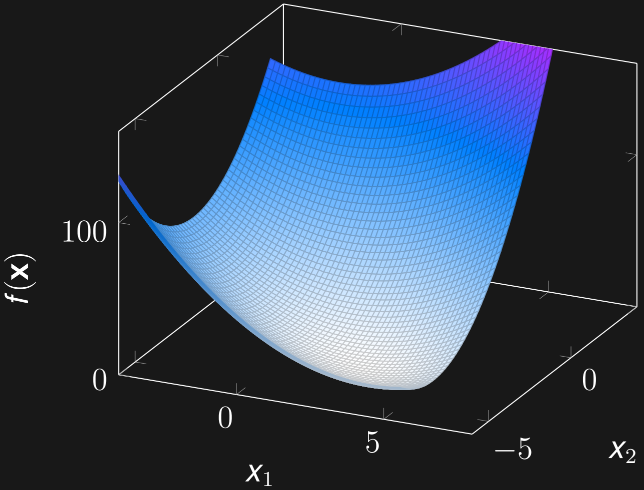
$$\mathbf{A} = \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix}, \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \text{ and } \mathbf{b} = \begin{pmatrix} 2 \\ -8 \end{pmatrix}.$$

Instead of solving $\mathbf{A}\mathbf{x} = \mathbf{b}$, the quadratic form, which is a function of $\mathbf{x}$ can be

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} - b^T\mathbf{x} + c$$

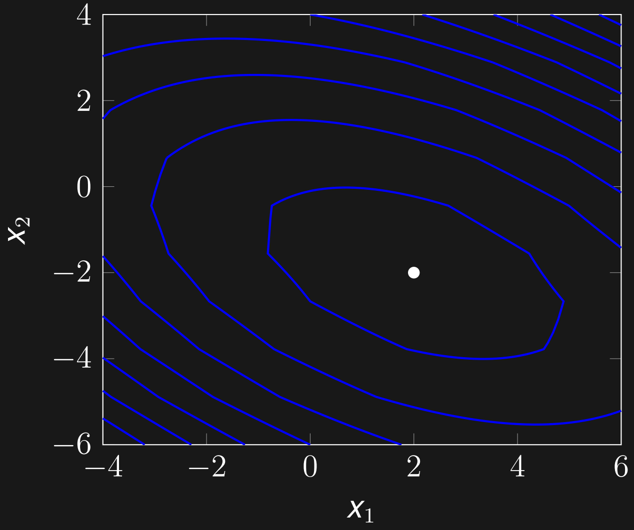
can be minimized to find the solution $\mathbf{x}$.

Plot of the quadratic form $f(\mathbf{x})$



Finding the minimal point of $\mathbf{x}$ corresponds to the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$.

Contour plot of the quadratic form $f(\mathbf{x})$



Gradient of the quadratic form

Definition of the gradient:

$$f'(\mathbf{x}) = \begin{pmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x}) \\ \frac{\partial}{\partial x_2} f(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial x_n} f(\mathbf{x}) \end{pmatrix}$$

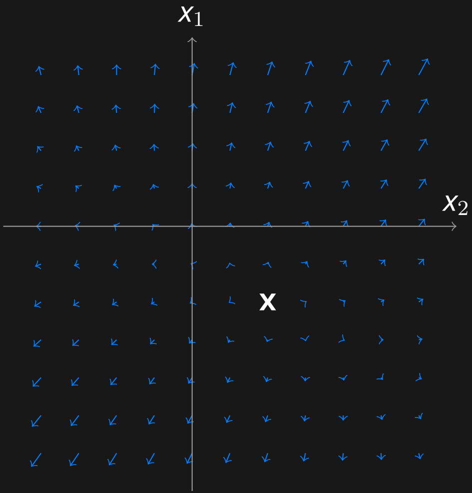
Applying a little bit of maths:

$$f'(\mathbf{x}) = \frac{1}{2}\mathbf{A}^T\mathbf{x} + \frac{1}{2}\mathbf{A}\mathbf{x} - \mathbf{b}$$

and for a symmetric matrix **A**, we get

$$f'(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b}$$

Gradient field



Since the gradient at the solution $\mathbf{x}$ is zero, we can set $f'(\mathbf{x})$ to zero to minimize $f(\mathbf{x})$.

The method of the steepest decent

- We chose an random point $\mathbf{x}_0$
- and slide down to the bottom of the quadratic form $f(\mathbf{x})$
- by taking a series of steps $\mathbf{x}_1, \mathbf{x}_2, \ldots$
- Each step we go to the direction which f decreases most which is the opposite of $f'(\mathbf{x}_i)$ which is

$$-f'(\mathbf{x}_i) = \mathbf{b} - \mathbf{A}\mathbf{x}_i$$

The method of the steepest decent

Error

$$\mathbf{e}_i = \mathbf{x}_i - \mathbf{x}$$

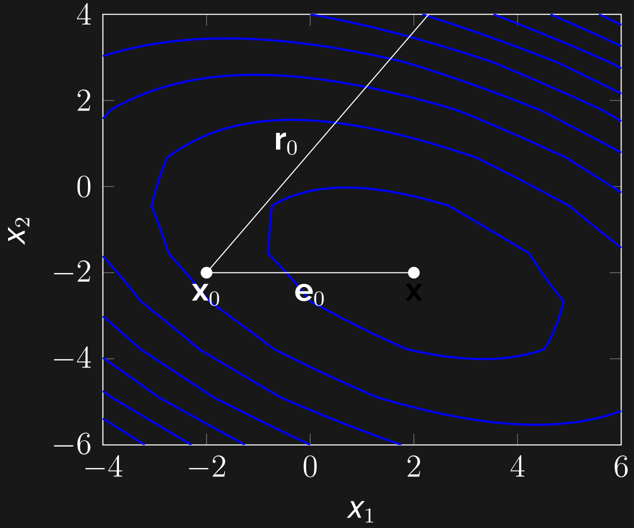
Defines how far way we are from the exact solution at iteration *i*.

Residual

$$\mathbf{r}_i = \mathbf{b} - \mathbf{A}\mathbf{x}_i = -f'(\mathbf{x}_i)$$

Defines how far away we are from the correct value for **b** in iteration *i*.

Visualization of the residual and error



How far to go along the residual vector?

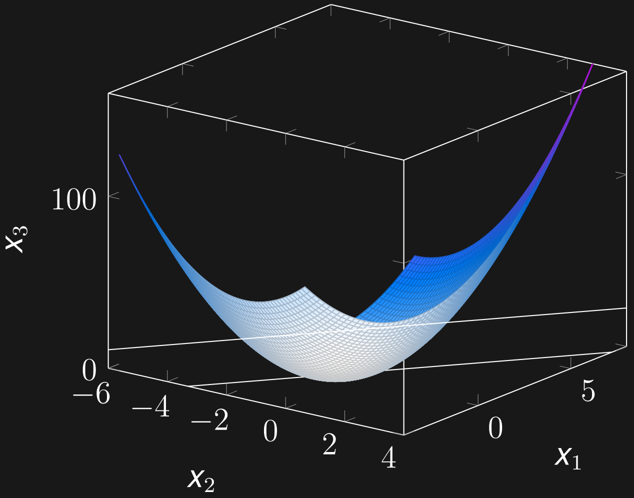
Line search

- We look at a starting point $\mathbf{x}_0 = [-2, -2]^T$
- from this point, we go along the direction of the steepest decent

$$\mathbf{x}_1 = \mathbf{x}_0 + \alpha \mathbf{r}_0$$

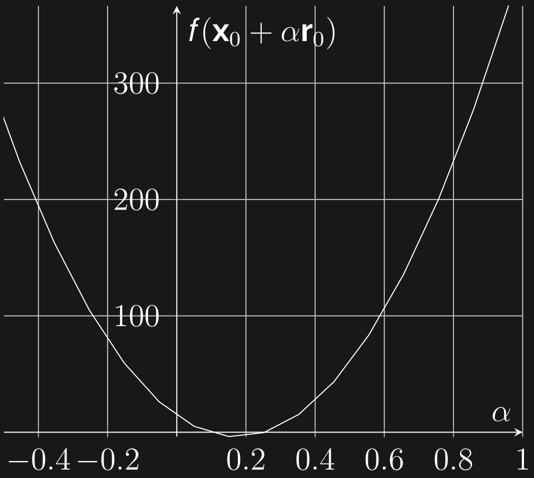
How large to chose α?

Two surfaces



We need to find the point on the intersection of the two surfaces which minimizes f.

Parabola by the intersection of the two surfaces



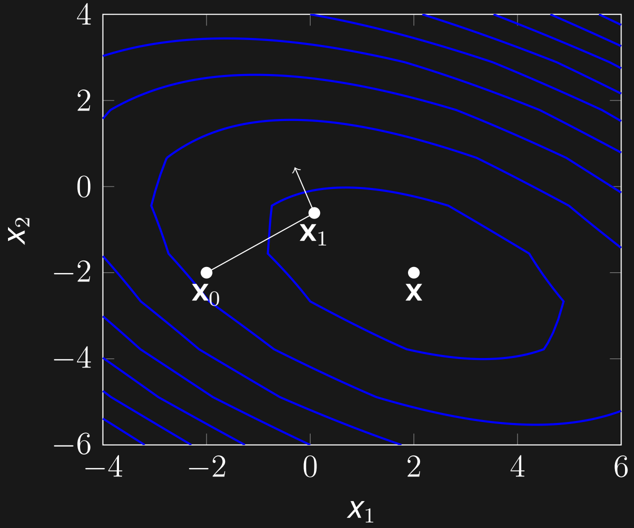
The minimum of this function is as $\frac{d}{d\alpha} f(\mathbf{x}_0 + \alpha \mathbf{r}_0) = 0$.

How to determine α?

Applying the chain rule: $\frac{d}{d\alpha}f(\mathbf{x}_0 + \alpha\mathbf{r}_0) = f'(\mathbf{x}_0 + \alpha\mathbf{r}_0)^T\mathbf{r}_0$.
This expression is zero, if the two vectors are orthogonal.

$$
\begin{aligned}
\mathbf{r}_1^T\mathbf{r}_0 &= 0 \\
(-\mathbf{A}\mathbf{x}_1)^T\mathbf{r}_0 &= 0 \\
(-\mathbf{A}(\mathbf{x}_0 + \alpha\mathbf{r}_0))^T\mathbf{r}_0 &= 0 \\
(\mathbf{b} - \mathbf{A}\mathbf{x}_0)^T\mathbf{r}_0 - \alpha(\mathbf{A}\mathbf{r}_0)^T\mathbf{r}_0 &= 0 \\
(\mathbf{b} - \mathbf{A}\mathbf{x}_0)^T\mathbf{r}_0 &= \alpha(\mathbf{A}\mathbf{r}_0)^T\mathbf{r}_0 \\
\mathbf{r}_0^T\mathbf{r}_0 &= \alpha\mathbf{r}_0^T(\mathbf{A}\mathbf{r}_0) \\
\alpha &= \frac{\mathbf{r}_0^T\mathbf{r}_0}{\mathbf{r}_0^T\mathbf{A}\mathbf{r}_0}
\end{aligned}
$$

Visualization of gradient of the previous step

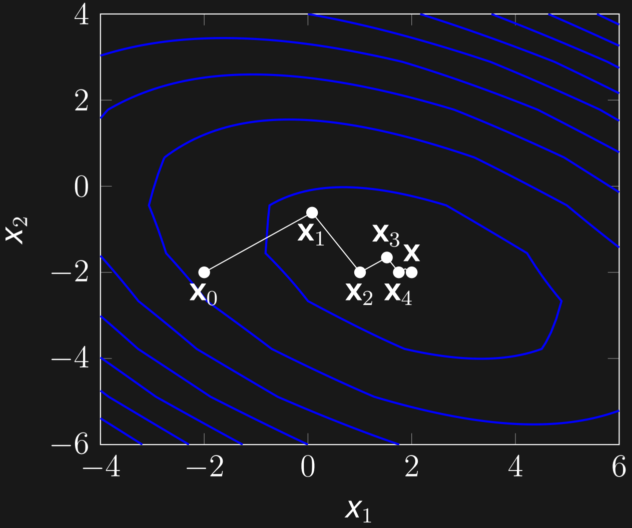


The gradient at $\mathbf{x}_1$ is orthogonal to $\mathbf{x}_0$.

Algorithm

1. $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$
2. If $|\mathbf{r}_0| < \epsilon$ return $\mathbf{x}_0$
3. $\mathbf{r}_i = \mathbf{b} - \mathbf{A}\mathbf{x}_i$
4. $\alpha_i = \frac{\mathbf{r}_0^T \mathbf{r}_0}{\mathbf{r}_0^T \mathbf{A}\mathbf{r}_0}$
5. $\mathbf{x}_{i+1} = \mathbf{x}_i \alpha_i \mathbf{r}_i$
6. If $|\mathbf{r}_i| < \epsilon$ return $\mathbf{x}_i$
7. Go to (3)

Visualization of the line search



The solution after five steps $\mathbf{x}_5 = [1.93832964, -2.]^T$.

Blaze Iterative

About BlazeIterative[1]

This is a set of iterative linear system solvers intended for use with the Blaze library, a high-performance C++ linear algebra library. The API is currently based on a tag-dispatch system to choose a particular algorithm.

Usage

```
#Install
tar -xvf blaze_iterative.gz
cd blaze_iterative
cp -r ./blaze_iterative /home/patrick/

#Compile
g++ -I/home/diehlpk/blaze
    -I/home/patrick/blaze_iterative BlazeTest.cpp
```

[1] https://github.com/STEllAR-GROUP/BlazeIterative

Conjugate gradient example

```
#include "BlazeIterative.hpp"

using namespace blaze;
using namespace blaze::iterative;

std::size_t N = 10;
DynamicMatrix<double,false> A(N,N, 0.0);
DynamicVector<double> b(N, 0.0);
DynamicVector<double> x1(N, 0.);

//Initialize the matrix

// Solve the system
ConjugateGradientTag tag;
auto x2 = solve(A,b,tag);
```

Available algorithms

Solvers

- Conjugate Gradient
- Preconditioned CG
- BiCGSTAB
- Generalized minimal residual method (GMRES),

Eigenvalues

- Lanczos

More details about solvers [1].

Summary

Summary

After this lecture, you should know

- Linear equation systems
- Conjugate gradient method
- BlazeIterative

Acknowledgment

- The very nice example for the introduction of the conjugate gradient method was adapted from:

  Shewchuk, Jonathan Richard. ”An introduction to the conjugate gradient method without the agonizing pain.” (1994).

References

References I

[1] Richard Barrett, Michael W Berry, Tony F Chan, James Demmel, June Donato, Jack Dongarra, Victor Eijkhout, Roldan Pozo, Charles Romine, and Henk Van der Vorst.
Templates for the solution of linear systems: building blocks for iterative methods, volume 43.
Siam, 1994.

[2] William L Briggs, Steve F McCormick, et al.
A multigrid tutorial, volume 72.
Siam, 2000.

[3] Magnus Rudolph Hestenes and Eduard Stiefel.
Methods of conjugate gradients for solving linear systems, volume 49.
NBS Washington, DC, 1952.