SOLVING EQUATIONS

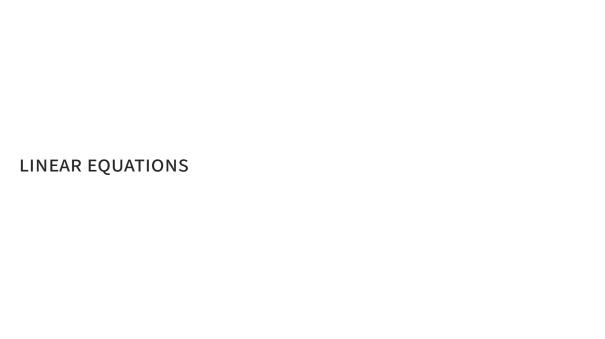
QUANTITATIVE ECONOMICS 2024

Piotr Żoch

November 6, 2024

INTRODUCTION

- Systems of linear equations.
- Nonlinear equations.



LINEAR SYSTEMS OF EQUATIONS

• One of the most common problems in scientific computation: solve

$$Ax = b$$
,

for **x**, where **A** is a square matrix and **b** is a vector.

- Seems like an easy problem, but it will teach us many things.
- Multiple specialized libraries for numerical linear algebra.

DIRECT METHODS

- Elementary operations:
 - mutliply a row by a scalar,
 - add a scalar multiple of a row to another row,
 - interchange two rows.
- Solve $\mathbf{A}\mathbf{x} = \mathbf{b}$ by using elementary row operations on the augmented matrix $[\mathbf{A} \mid \mathbf{b}]$.
- Transform A into a reduced row echelon form.

DIRECT METHODS

- Two step procedure:
 - Forward elimination.

- Backward elimination.

FLOATING POINT NUMBERS

- Forward elimination: to deal with the first column we need n^2 operations, for the second $n^2 1$, for the third $n^2 2$ and so on.
- Backward elimination: to deal with the last column we need n operations, for the second to last n-1, for the third to last n-2 and so on.
- Forward elimination is $O(n^3)$, backward elimination is $O(n^2)$.

TRIANGULAR SYSTEMS

Lower triangular system:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

can be solved using forward elimination, starting from the top

$$y_i = b_i - \sum_{i=1}^{i-1} l_{ij} y_j$$
.

UPPER TRIANGULAR SYSTEMS

Upper triangular system:

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

can be solved using backward elimination, starting from the bottom

$$x_i = \frac{1}{u_{ij}} \left(y_i - \sum_{j=i+1}^n u_{ij} x_j \right).$$

Suppose we can write

$$A = LU$$

where **L** is a lower triangular matrix and **U** is an upper triangular matrix.

We have

$$L(Ux) = b \rightarrow Ly = b$$

which we can solve for **y** using forward elimination.

We then solve

$$\mathbf{U}\mathbf{x} = \mathbf{y}$$

for **x** using backward elimination.

- This is known as Gaussian elimination.
 - 1. Compute L and U.
 - 2. Solve $\mathbf{L}\mathbf{y} = \mathbf{b}$ for \mathbf{y} using forward elimination.
 - 3. Solve **Ux** = **y** for **x** using backward elimination.
- Step 1. is known as LU decomposition.
- Nice thing: we can keep **L** and **U** and recycle them for different **b**.
- How to perform the decomposition?

MATRIX MULTIPLICATION BY OUTER PRODUCTS

- Write the columns of **A** as a_1, \ldots, a_n .
- Write the rows of **B** as $\mathbf{b}_1^{\mathsf{T}}, \dots, \mathbf{b}_n^{\mathsf{T}}$.
- We have

$$\mathbf{AB} = \sum_{k=1}^{n} \mathbf{a}_{k} \mathbf{b}_{k}^{\top}.$$

 Useful: for triangular matrices L, U only the first outer product contributes to the first row and the first column of LU

$$\mathbf{e}_1^{\mathsf{T}} \sum_{k=1}^n \mathbf{l}_k \mathbf{u}_k^{\mathsf{T}} = l_{11} \mathbf{u}_1^{\mathsf{T}}, \quad \left(\sum_{k=1}^n \mathbf{l}_k \mathbf{u}_k^{\mathsf{T}}\right) \mathbf{e}_1 = u_{11} \mathbf{l}_1.$$

LU FACTORIZATION WITHOUT PIVOTING

Algorithm LU Factorization without Pivoting

```
Require: Matrix \mathbf{A} \in \mathbb{R}^{n \times n}

1: \mathbf{for} \ j = 1 \ \mathbf{to} \ n \ \mathbf{do}

2: \mathbf{for} \ i = j + 1 \ \mathbf{to} \ n \ \mathbf{do}

3: a_{ij} = \frac{a_{ij}}{a_{jj}}

4: \mathbf{for} \ k = j + 1 \ \mathbf{to} \ n \ \mathbf{do}

5: a_{jk} = a_{jk} - a_{ij}a_{jk}

6: \mathbf{end} \ \mathbf{for}

7: \mathbf{end} \ \mathbf{for}

8: \mathbf{end} \ \mathbf{for}
```

- This algorithm uses A matrix to store L and U.
- Problem when $a_{ij} = 0$ at any step -

SOLVING THE SYSTEM

We need

$$\sum_{j=1}^{n} \sum_{i=j+1}^{n} \left(1 + \sum_{k=j+1}^{n} 2 \right) = \frac{2}{3} n^3 - \frac{1}{2} n^2 - \frac{1}{6} n$$

operations to perform the factorization.

We then need

$$\sum_{i=1}^{n} \left(2 + \sum_{j=1}^{i-1} 2 \right) = n^2 + n$$

operations for forward and backward substitution each.

LU decomposition is the most costly step.

SOLVING THE SYSTEM

We need

$$\sum_{j=1}^{n} \sum_{i=j+1}^{n} \left(1 + \sum_{k=j+1}^{n} 2 \right) = \frac{2}{3} n^3 - \frac{1}{2} n^2 - \frac{1}{6} n$$

operations to perform the factorization.

We then need

$$\sum_{i=1}^{n} \left(2 + \sum_{j=1}^{i-1} 2 \right) = n^2 + n$$

operations for forward and backward substitution each.

LU decomposition is the most costly step.

SOLVING THE SYSTEM

- In practice we use a similar method, but with pivoting
- PLU factorization:

$$\tilde{\mathbf{A}} = \mathbf{L}\mathbf{U},$$

where $\tilde{\mathbf{A}}$ is a matrix \mathbf{A} with its rows permuted.

- It works if and only if A is non-singular.
- Asymptotically uses the same number of operations and LU without pivoting.

NORMS

- A vector norm is a function $\|\cdot\| : \mathbb{R}^n \to \mathbb{R}$ that satisfies:
 - 1. $\|\mathbf{x}\| \geq 0$,
 - $2. \|\mathbf{x}\| = 0 \iff \mathbf{x} = \mathbf{0},$
 - 3. $\|a\mathbf{x}\| = |a| \|\mathbf{x}\|$,
 - 4. $\|\mathbf{x} + \mathbf{y}\| \le \|\mathbf{x}\| + \|\mathbf{y}\|$,

for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and $a \in \mathbb{R}$.

• Common vector norms: $\ell_1, \ell_2, \ell_\infty$:

$$\|\mathbf{x}\|_{1} = \sum_{i=1}^{n} |x_{i}|, \quad \|\mathbf{x}\|_{2} = \sqrt{\sum_{i=1}^{n} x_{i}^{2}}, \quad \|\mathbf{x}\|_{\infty} = \max_{i=1,...,n} |x_{i}|.$$

NORMS

- For matrices we have matrix norms.
- A Frobenius norm is

$$\|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2}.$$

- Imagine representing a matrix as a vector with columns stacked on top of each other.
- An induced matrix norm is

$$\|\mathbf{A}\|_p = \max_{\|\mathbf{x}\|_p=1} \|\mathbf{A}\mathbf{x}\|_p$$
.

• In Julia: norm(A) is the Frobenius norm, opnorm(A,p) is the induced norm.

NORMS

- We have
 - 1. $\|\mathbf{A}\mathbf{x}\| \leq \|\mathbf{A}\| \|\mathbf{x}\|$,
 - 2. $\|AB\| \le \|A\| \|B\|$,
 - 3. for a square matrix, $\|\mathbf{A}^k\| \le \|\mathbf{A}\|^k$ for any integer $k \ge 0$.
- Two common matrix norm are the 1-norm and the ∞-norm:

$$\|\mathbf{A}\|_1 = \max_{j=1,\dots,n} \sum_{i=1}^m |a_{ij}|, \quad \|\mathbf{A}\|_{\infty} = \max_{i=1,\dots,m} \sum_{i=1}^n |a_{ij}|.$$

Consider the perturbed system

$$A(x+h)=b+d.$$

• The condition number is the relative change in the solution divided by the relative change in the data:

$$\kappa = \frac{\|\mathbf{h}\| / \|\mathbf{x}\|}{\|\mathbf{d}\| / \|\mathbf{b}\|} = \frac{\|\mathbf{h}\| \|\mathbf{b}\|}{\|\mathbf{d}\| \|\mathbf{x}\|}.$$

• Note that $\mathbf{h} = \mathbf{A}^{-1}\mathbf{d}$ so

$$\|\mathbf{h}\| \le \|\mathbf{A}^{-1}\| \|\mathbf{d}\|.$$

• Use $\|\mathbf{h}\| \le \|\mathbf{A}^{-1}\| \|\mathbf{d}\|$ to write

$$\frac{\|h\| \|b\|}{\|d\| \|x\|} \le \frac{\|A^{-1}\| \|d\| \|A\| \|x\|}{\|d\| \|x\|} = \|A^{-1}\| \|A\|.$$

- We can prove that inequality is tight.
- The matrix condition number of an invertible square matrix A is

$$\kappa(\mathbf{A}) = \|\mathbf{A}^{-1}\| \|\mathbf{A}\|.$$

• If $\mathbf{A}(\mathbf{x} + \Delta \mathbf{x}) = \mathbf{b} + \Delta \mathbf{b}$ then

$$\frac{\left\|\Delta \boldsymbol{x}\right\|}{\left\|\boldsymbol{x}\right\|} \leq \kappa \left(\boldsymbol{A}\right) \frac{\left\|\Delta \boldsymbol{b}\right\|}{\left\|\boldsymbol{b}\right\|}.$$

- The condition number is a measure of how sensitive the solution is to changes in the data.
- We can derive a similar result for perturbed A.
- The condition number is at least equal to 1.
- A condition number of 10^k means that we lose k digits of precision.

- Suppose that we compute a "solution" $\tilde{\mathbf{x}}$ to the system $\mathbf{A}\mathbf{x} = \mathbf{b}$.
- We would like to compare $\tilde{\mathbf{x}}$ to the true solution \mathbf{x} but we do not know \mathbf{x} .
- We can calculate the residual

$$r = b - A\tilde{x}$$

•

We have

$$\frac{\left\|\mathbf{x} - \tilde{\mathbf{x}}\right\|}{\|\mathbf{x}\|} \le \kappa \left(\mathbf{A}\right) \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}.$$

- We saw that Gaussian elimination is $\mathcal{O}(n^3)$.
- This is prohibitive for large *n* (unless a matrix has a special structure).
- But matrix-vector multiplication is $O(n^2)$.
- In some cases we can apply repeated matrix-vector multiplication to solve the system.
- We call these iterative methods.

JACOBI METHOD

- Suppose we want to solve $\mathbf{A}\mathbf{x} = \mathbf{b}$.
- This can be written as

$$\sum_{j=1}^{n} a_{ij} x_j = b_i, \quad \text{or} \quad x_i = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij} x_j \right).$$

• Start from some initial $\mathbf{x}^{(0)}$ and iterate:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij} x_j^{(k)} \right)$$

until $\mathbf{x}^{(k+1)}$ is close enough to $\mathbf{x}^{(k)}$.

GAUSS-SEIDEL METHOD

We can also write

$$x_i = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j - \sum_{j=i+1}^{n} a_{ij} x_j \right).$$

• The Gauss-Seidel method uses the newest values of x_i:

$$x_i^{(k+1)} = \frac{1}{a_{ij}} \left(b_i - \sum_{i=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{i=i+1}^{n} a_{ij} x_j^{(k)} \right).$$

• Rewrite $\mathbf{A} = \mathbf{P} - \mathbf{N}$ so that the system is

$$Px = Nx + b.$$

An iterative method is

$$\mathbf{Px}^{(k+1)} = \left(\mathbf{Nx}^{(k)} + \mathbf{b}\right).$$

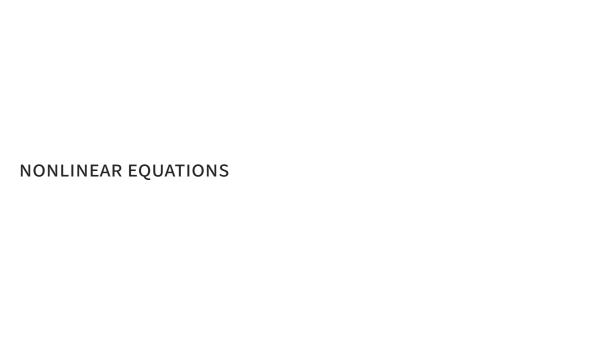
- P is called a preconditioner
- Jacobi and Gauss-Seidel differ in the choice of P.
- Since $\mathbf{x}^{k+1} = \mathbf{P}^{-1} \left(\mathbf{N} \mathbf{x}^{(k)} + \mathbf{b} \right)$ a good preconditioner should be easy to invert.

- Why do we call **P** a preconditioner?
- Suppose we have a system $\mathbf{A}\mathbf{x} = \mathbf{b}$.
- The condition number is $\kappa(\mathbf{A})$.
- Suppose we have a preconditioned system $P^{-1}Ax = P^{-1}b$.
- The condition number is $\kappa(\mathbf{P}^{-1}\mathbf{A})$.
- If $\mathbf{P} \approx \mathbf{A}^{-1}$, then $\kappa \left(\mathbf{P}^{-1} \mathbf{A} \right) \approx 1$.

- Iterative methods do not always converge.
- They are guaranteed to converge if A is diagonally dominant:

$$|a_{ii}| > \sum_{i \neq i} |a_{ij}|.$$

 There are better methods than Jacobi and Gauss-Seidel - the idea is to choose P so that the convergence is faster.



NONLINEAR EQUATIONS

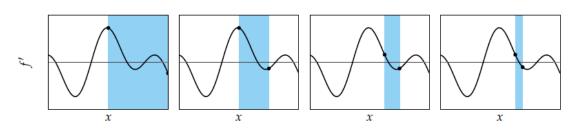
We want to find a solution x* to

$$f(x) = 0.$$

- We call x* a root of f.
- Usually we cannot get the exact solution in a finite number of steps.
- We will focus on $f : \mathbb{R} \to \mathbb{R}$.
- Even simple polynomial equations can have no closed-form solution:

$$x^5 + 2x^2 + 1 = 0.$$

- Suppose we have a continuous function $f : \mathbb{R} \to \mathbb{R}$.
- We do not require it to be differentiable.
- We also have two points a < b such that f(a)f(b) < 0 (opposite signs).
- We call [a, b] a bracket.
- By the intermediate value theorem there exists a point x^* such that $f(x^*) = 0, x^* \in (a, b)$.
- Evaluate f(m) where $m = \frac{a+b}{2}$.
 - If f(m) = 0 we are done.
 - − If f(m)f(a) < 0 then $x^* \in (a, m)$. Use m as the new b.
 - If f(m)f(b) < 0 then x^* ∈ (m,b). Use m as the new a.
- Repeat until b a is small enough.



Source: Kochenderfer and Wheeler (2019)

- Good: bisection is *guaranteed* to converge to a root.
- Bad: it is slow. But how slow?
- If there are multiple roots, it will find just one of them this is a general problem with root-finding algorithms.

CONVERGENCE

• A sequence $\{x_1, x_2, ...\}$ converges to x^* with order p, if there exists a constant C such that

$$\left|x_{k+1}-x^*\right|\leq C\left|x_k-x^*\right|^p.$$

for all *k* large enough.

- We call r the rate of convergence.
- A method is locally convergent if the sequence converges to x^* for x_0 close enough to x^* .
- A method is globally convergent if the sequence converges to x^* for any x_0 .

- The initial bracket in the bisection method is $I_0 = [a, b]$. Its length is b a.
- The bracket after the first iteration is either $I_1 = \left[a, \frac{a+b}{2} \right]$ or $I_1 = \left[\frac{a+b}{2}, b \right]$. Its length is $\frac{b-a}{2}$.
- The bracket after the k-th iteration has length $\frac{b-a}{2^k}$.
- We have

$$\left|x_{k}-x^{*}\right| \leq \left(\frac{1}{2}\right)\left|x_{k-1}-x^{*}\right|$$

• The order of convergence is p = 1 and the rate of convergence is $r = \frac{1}{2}$.

BISECTION METHOD

- We add one bit of precision in each iteration.
- To get one digit of precision we need to perform \approx 3.3 iterations (since $\log_2 10 \approx$ 3.3).
- If we want to have $|x^k x^*| \le \gamma$, we need to perform

$$k = \log_2\left(\frac{|b-a|}{\gamma}\right)$$

iterations.

The above follows from

$$\left|x^{k}-x^{*}\right|\leq 2^{-k}\left|b-a\right|.$$

BISECTION METHOD

- Bisection has p = 1 and $r = \frac{1}{2}$. If p = 1 and r < 1 the order of convergence is called linear.
- If p = 1 but $r_k < 1$ and $\rho_k \to 0$ as $k \to \infty$ the order of convergence is called superlinear.
- If p = 2 the order of convergence is called quadratic.
- If p = 3 the order of convergence is called cubic...
- The order of convergence does not have to be an integer.

- The bisection method did not use much information about the function f.
- We can use more information to design faster methods.
- Consider a Taylor expansion of $f(x^*)$ around x:

$$f(x^*) = f(x) + f'(x)(x - x^*) + \frac{1}{2}f''(\xi)(x - x^*)^2, \quad \xi \in (x^*, x)$$

• Use $f(x^*) = 0$ to solve for x^* :

$$x^* = x - \frac{f(x)}{f'(x)} + o(|x^* - x|).$$

• This suggests that x^* is close to $x - \frac{f(x)}{f'(x)}$.

• Start with x_0 and consider the sequence given by

$$x_{k+1} = \frac{f(x_k)}{f'(x_k)}.$$

- This is the Newton method. Also known as the Newton-Raphson method.
- Be careful: the method can diverge. Easy to see if f'(x) = 0.

- What is the order of convergence of the Newton method?
- We have $x_k = x^* + e_k$, where e_k is the error at the k-th iteration.
- We have

$$\begin{split} e_{k+1} &= e_k - \frac{f(x_k)}{f'(x_k)} \\ &= e_k - \frac{f(x^* + e_k)}{f'(x^* + e_k)} \\ &= \frac{\frac{1}{2}f''(x^*)e_k^2 + \frac{1}{3}f'''(x^*)\left(e_k^3 + o(e_k^3)\right)}{f'(x^*) + f''(x^*)e_k^2 + o(e_k)} \\ &= \frac{f''(x^*)}{2f'(x^*)}e_k^2 + o(e_k^2), \end{split}$$

if $f''(x^*) \neq 0$. Note that e_k is raised to the power of 2.

- The order of convergence is p = 2, so it is quadratic.
- The number of correct digits approximately doubles in each iteration.
- Good guess: 6-7 iterations to get an answer within machine precision.
- Note: if x^* is a double root, then $e_{k+1} \approx \frac{1}{2}e_k$ linear convergence.

- Good: the Newton method is fast.
- Bad: you need a good guess, not guaranteed to converge.
- You also need to calculate the derivative at each x_k . How to do this?
- *f* has to be sufficiently smooth (we used the Taylor expansion to show quadratic convergence).

SECANT METHOD

- Insteady of calculating the derivative, we can approximate it.
- Suppose we have two points x_k and x_{k-1} .
- We can approximate the derivative at x_k as

$$f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}.$$

The secant method is

$$x_{k+1} = x_k - f(x_k) \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}.$$

- The order of convergence is $p \approx 1.6$.
- Requires two initial guesses.

SECANT METHOD

- $p \approx 1.6$ is between linear and quadratic convergence. Seems worse than Newton.
- In each iteration of Newton we use $f'(x_k)$ and $f(x_k)$.
- In each iteration of the secant method we use $f(x_k)$ and $f(x_{k-1})$, but we already calculated $f(x_{k-1})$ in the previous iteration.
- If function evaluations are used to measure computational work, the secant iteration converges more rapidly than Newton's method.

BRENT METHOD

- Bisection is slow, but guaranteed to converge.
- Newton is fast, but requires a good guess.
- The Brent method (Dekker-Brent) combines the two:
 - 1. Start with a bracket.
 - 2. Do a step of Newton / secant to get x_k . If it is within the bracket, accept it. Otherwise do bisection.
 - 3. Update the bracket using the new point.
 - 4. Repeat until convergence.
- The Brent method uses an inverse quadratic interpolation to get an approximate f'.

MULTIDIMENSIONAL METHODS

- Newton's method can be extended to multiple dimensions; $f : \mathbb{R}^n \to \mathbb{R}^n$.
- Suppose we want to solve f(x) = 0.
- The Newton method is

$$\mathbf{x}_{k+1} = \mathbf{x}_k - [\mathbf{J}(\mathbf{x}_k)]^{-1} \mathbf{f}(\mathbf{x}_k).$$

• **J** is the Jacobian matrix of *f*:

$$\mathbf{J}_{ij}(\mathbf{x}) = \frac{\partial \mathbf{f}_i(\mathbf{x})}{\partial x_i}.$$

MULTIDIMENSIONAL METHODS

- In practice we do not calculate the inverse of the Jacobian.
- We solve

$$\mathbf{J}(\mathbf{x}_k)\mathbf{s}_k = -\mathbf{f}(\mathbf{x}_k).$$

and update

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k.$$

• Challenge: it is expensive to calculate the Jacobian.

BROYDEN METHOD

Note that what we do is:

$$\mathbf{A}_k \mathbf{s}_k = -\mathbf{f}(\mathbf{x}_k).$$
 $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k.$

- We had $\mathbf{A}_k = \mathbf{J}(\mathbf{x}_k)$. But there are other ways to choose \mathbf{A}_k .
- One possible choice is

$$\mathbf{A}_{k+1} = \mathbf{A}_k + \frac{1}{\mathbf{s}_k^{\top} \mathbf{s}_k} \left[\mathbf{f}(\mathbf{x}_{k+1}) - \mathbf{f}(\mathbf{x}_k) - \mathbf{A}_k \mathbf{s}_k \right] \mathbf{s}_k^{\top}.$$

- This is the Broyden method.
- Under some conditions the Broyden method converges superlinearly (but \mathbf{A}_k is not guaranteed to converge to the Jacobian).

LEVENBERG STEP

- Problem: it is possible to diverge.
- One way to prevent divergence is to add a Levenberg step.
- Check if an usual Newton step would lead to an improvement.
- If not, go in a direction that is guaranteed to an improvement.

$$\left(\mathbf{A}_k^{\top}\mathbf{A}_k + \lambda \mathbf{I}\right)\mathbf{s}_k = -\mathbf{A}_k^{\top}\mathbf{f}(\mathbf{x}_k).$$

• Adjust λ to ensure that the function value gets closer to zero.