



Conjugate gradients method

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Strongly convex quadratics

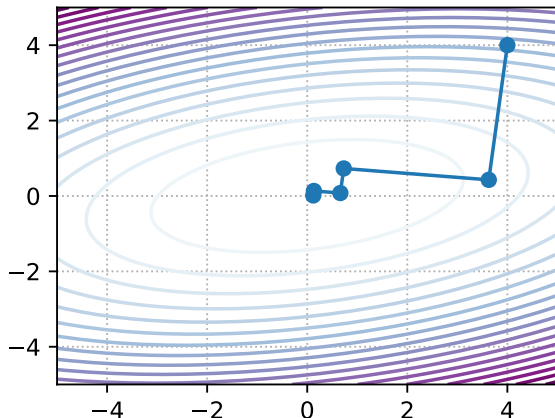
Consider the following quadratic optimization problem:

Optimality conditions

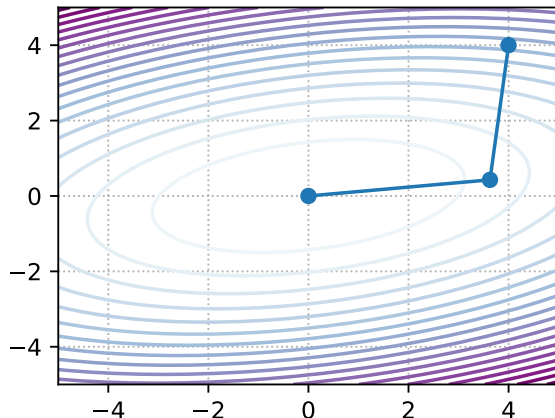
$$\min_{x \in \mathbb{R}^n} f(x) = \min_{x \in \mathbb{R}^n} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}_{++}^n. \quad (1)$$

$$A x^* = b$$

Steepest Descent



Conjugate Gradient



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:

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

🔥 Optimal value for quadratics

$$\nabla f(x_k)^T A(x_k - \alpha \nabla f(x_k)) - \nabla f(x_k)^T b = 0 \quad \alpha_k = \frac{\nabla f(x_k)^T \nabla f(x_k)}{\nabla f(x_k)^T A \nabla f(x_k)}$$

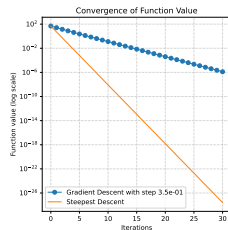
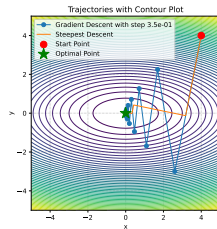


Figure 1: Steepest Descent

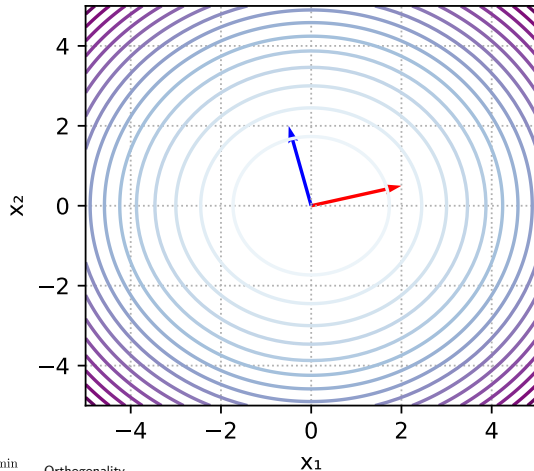
Open In Colab

Conjugate directions. A -orthogonality.

v_1 and v_2 are orthogonal

$$v_1^T v_2 = 0.00$$

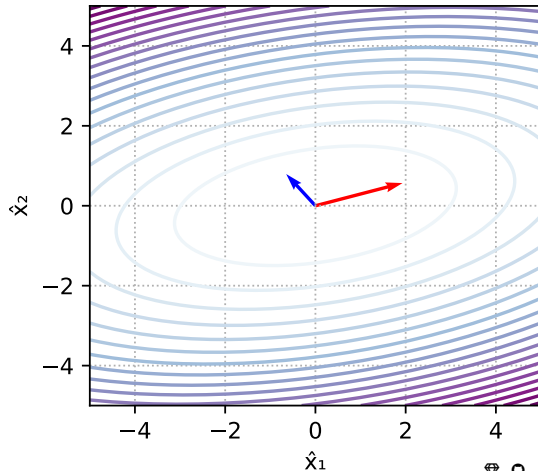
$$v_1^T A v_2 = 1.19$$



\hat{v}_1 and \hat{v}_2 are A -orthogonal

$$\hat{v}_1^T \hat{v}_2 = -0.80$$

$$\hat{v}_1^T A \hat{v}_2 = -0.00$$



Conjugate directions. A -orthogonality.

Suppose, we have two coordinate systems and some quadratic function $f(x) = \frac{1}{2}x^T Ix$ looks just like on the left part of Figure 2, while in other coordinates it looks like $f(\hat{x}) = \frac{1}{2}\hat{x}^T A\hat{x}$, where $A \in \mathbb{S}_{++}^n$.

$$\frac{1}{2}x^T Ix$$

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Since $A = Q\Lambda Q^T$:

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A -orthogonal vectors

Vectors $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$ are called A -orthogonal (or A -conjugate) if

$$x^T Ay = 0 \quad \Leftrightarrow \quad x \perp_A y$$

When $A = I$, A -orthogonality becomes orthogonality.

Gram–Schmidt process

Input: n linearly independent vectors u_0, \dots, u_{n-1} .

Output: n linearly independent vectors, which are pairwise orthogonal d_0, \dots, d_{n-1} .

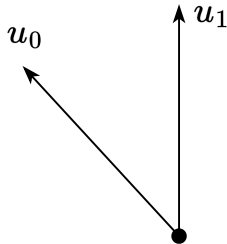


Figure 3: Illustration of Gram-Schmidt orthogonalization process

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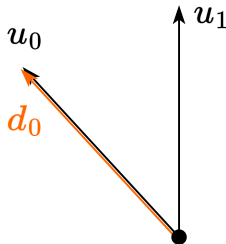


Figure 4: Illustration of Gram-Schmidt orthogonalization process

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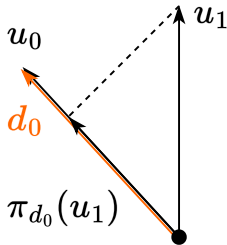


Figure 5: Illustration of Gram-Schmidt orthogonalization process

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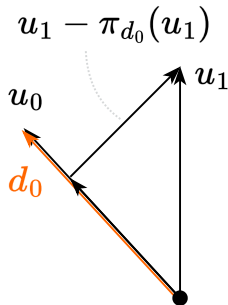


Figure 6: Illustration of Gram-Schmidt orthogonalization process

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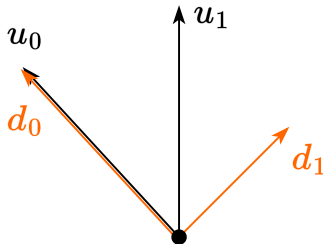
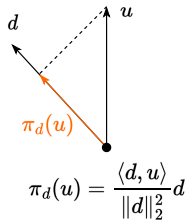
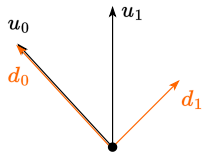


Figure 7: Illustration of Gram-Schmidt orthogonalization process

Gram–Schmidt process

Input: n linearly independent vectors u_0, \dots, u_{n-1} .

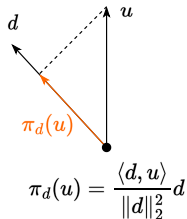
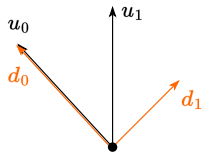


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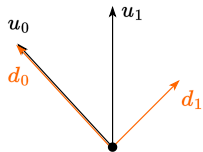
$$d_0 = u_0$$



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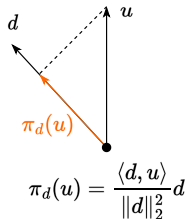
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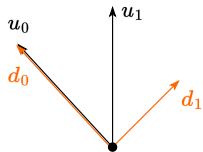
$$d_1 = u_1 - \pi_{d_0}(u_1)$$



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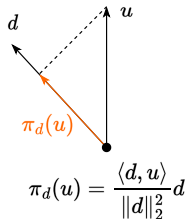
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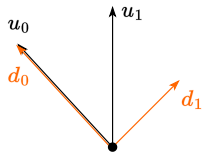
$$d_2 = u_2 - \pi_{d_0}(u_2) - \pi_{d_1}(u_2)$$



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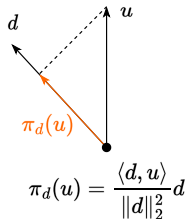


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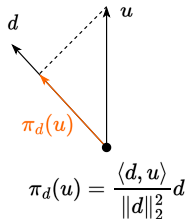
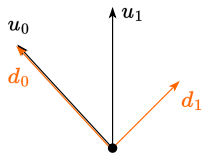
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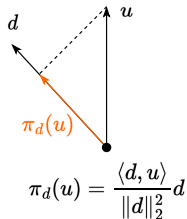
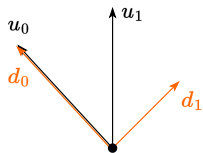
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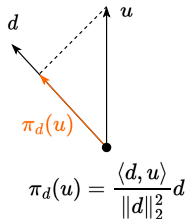
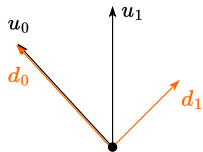
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$$d_k = u_k - \sum_{i=0}^{k-1} \pi_{d_i}(u_k)$$

$$d_k = u_k + \sum_{i=0}^{k-1} \beta_{ik} d_i \quad \beta_{ik} = -\frac{\langle d_i, u_k \rangle}{\langle d_i, d_i \rangle} \quad (2)$$

General idea

- In an isotropic $A = I$ world, the steepest descent starting from an arbitrary point in any n orthogonal linearly independent directions will converge in n steps in exact arithmetic. We attempt to construct the same procedure in the case $A \neq I$ using the concept of A -orthogonality.

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$$x^* = x_0 + \sum_{i=0}^{n-1} \alpha_i d_i \quad x^* - x_0 = \sum_{i=0}^{n-1} \alpha_i d_i$$

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- We will prove, that α_i and d_i could be selected in a very efficient way (Conjugate Gradient method).

Idea of Conjugate Directions (CD) method

Thus, we formulate an algorithm:

1. Let $k = 0$ and $x_k = x_0$, count $d_k = d_0 = -\nabla f(x_0)$.

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5. Repeat steps 2-4 until n directions are built, where n is the dimension of space (dimension of x).

Conjugate Directions (CD) method

i Lemma 1. Linear independence of A -conjugate vectors.

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- Note also, that since $x_{k+1} = x_0 + \sum_{i=1}^k \alpha_i d_i$, we have

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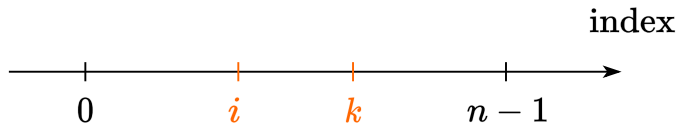
Proof

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Multiply both sides by $-d_i^T A$.

$$-d_i^T A e_k = \sum_{j=k}^{n-1} \alpha_j d_i^T A d_j = 0$$



Thus, $d_i^T r_k = 0$ and residual r_k is orthogonal to all previous directions d_i for the CD method.

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- It is literally the Conjugate Direction method, where we have a special (effective) choice of d_0, \dots, d_{n-1} .

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CG = CD + r_0, \dots, r_{n-1} as starting vectors for Gram-Schmidt + A -orthogonality.

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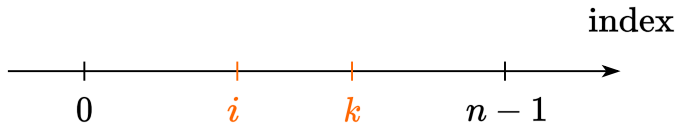
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Multiply both sides of (9) by $r_k^T \cdot$ for some index k :

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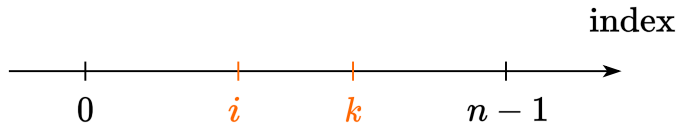
$$d_i = u_i + \sum_{j=0}^{k-1} \beta_{ji} d_j \quad \beta_{ji} = -\frac{\langle d_j, u_i \rangle_A}{\langle d_j, d_j \rangle_A} \quad (9)$$

Then, we use residuals as starting vectors for the process and $u_i = r_i$.

$$d_i = r_i + \sum_{j=0}^{k-1} \beta_{ji} d_j \quad \beta_{ji} = -\frac{\langle d_j, r_i \rangle_A}{\langle d_j, d_j \rangle_A} \quad (10)$$

If $j < i < k$, we have the lemma 4 with $d_i^T r_k = 0$ and $d_j^T r_k = 0$. We have:

$$r_k^T u_i = 0 \quad \text{for CD} \quad r_k^T r_i = 0 \quad \text{for CG}$$



Lemms for convergence

Moreover, if $k = i$:

$$r_k^T d_k = r_k^T u_k + \sum_{j=0}^{k-1} \beta_{jk} r_k^T d_j$$

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$$r_{k+1} = -A e_{k+1} = -A(e_k + \alpha_k d_k) = -A e_k - \alpha_k A d_k = r_k - \alpha_k A d_k$$

Finally, all these above lemmas are enough to prove, that $\beta_{ji} = 0$ for all i, j , except the neighboring ones.

Gram-Schmidt process in CG method

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$$\beta_{ji} = -\frac{\langle d_j, u_i \rangle_A}{\langle d_j, d_j \rangle_A}$$

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$$\beta_{ji} = -\frac{\langle d_j, u_i \rangle_A}{\langle d_j, d_j \rangle_A} = -\frac{d_j^T A u_i}{d_j^T A d_j} = -\frac{d_j^T A r_i}{d_j^T A d_j} = -\frac{r_i^T A d_j}{d_j^T A d_j}.$$

Consider the scalar product $\langle r_i, r_{j+1} \rangle$ using (12):

$$\langle r_i, r_{j+1} \rangle = \langle r_i, r_j - \alpha_j A d_j \rangle = \langle r_i, r_j \rangle - \alpha_j \langle r_i, A d_j \rangle$$

$$\alpha_j \langle r_i, A d_j \rangle = \langle r_i, r_j \rangle - \langle r_i, r_{j+1} \rangle$$

1. If $i = j$: $\alpha_i \langle r_i, A d_i \rangle = \langle r_i, r_i \rangle - \langle r_i, r_{i+1} \rangle = \langle r_i, r_i \rangle$. This case is not of interest due to the GS process.
2. Neighboring case $i = j + 1$: $\alpha_j \langle r_i, A d_j \rangle = \langle r_i, r_{i-1} \rangle - \langle r_i, r_i \rangle = -\langle r_i, r_i \rangle$
3. For any other case: $\alpha_j \langle r_i, A d_j \rangle = 0$, because all residuals are orthogonal to each other.

Finally, we have a formula for $i = j + 1$:

$$\beta_{ji} = -\frac{r_i^T A d_j}{d_j^T A d_j} = \frac{1}{\alpha_j} \frac{\langle r_i, r_i \rangle}{d_j^T A d_j} = \frac{d_j^T A d_j}{d_j^T r_j} \frac{\langle r_i, r_i \rangle}{d_j^T A d_j} = \frac{\langle r_i, r_i \rangle}{\langle r_j, r_j \rangle} = \frac{\langle r_i, r_i \rangle}{\langle r_{i-1}, r_{i-1} \rangle}$$

And for the direction

$$d_{k+1} = r_{k+1} + \beta_{k,k+1} d_k, \quad \beta_{k,k+1} = \beta_k = \frac{\langle r_{k+1}, r_{k+1} \rangle}{\langle r_k, r_k \rangle}.$$

Conjugate gradients method

$$\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$$

if \mathbf{r}_0 is sufficiently small, then return \mathbf{x}_0 as the result

$$\mathbf{d}_0 := \mathbf{r}_0$$

$$k := 0$$

repeat

$$\alpha_k := \frac{\mathbf{r}_k^\top \mathbf{r}_k}{\mathbf{d}_k^\top \mathbf{A} \mathbf{d}_k}$$

$$\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{d}_k$$

$$\mathbf{r}_{k+1} := \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{d}_k$$

if \mathbf{r}_{k+1} is sufficiently small, then exit loop

$$\beta_k := \frac{\mathbf{r}_{k+1}^\top \mathbf{r}_{k+1}}{\mathbf{r}_k^\top \mathbf{r}_k}$$

$$\mathbf{d}_{k+1} := \mathbf{r}_{k+1} + \beta_k \mathbf{d}_k$$

$$k := k + 1$$

end repeat

return \mathbf{x}_{k+1} as the result

Convergence

Theorem 1. If matrix A has only r different eigenvalues, then the conjugate gradient method converges in r iterations.

Theorem 2. The following convergence bound holds

$$\|x_k - x^*\|_A \leq 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k \|x_0 - x^*\|_A,$$

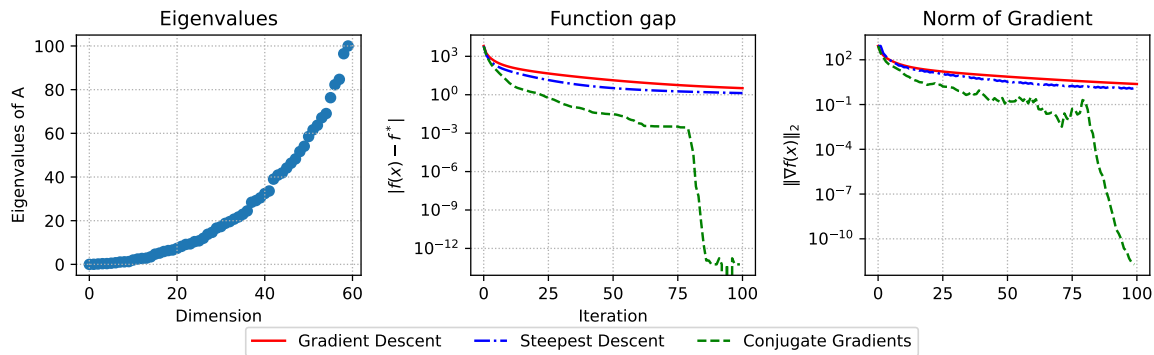
where $\|x\|_A^2 = x^\top A x$ and $\kappa(A) = \frac{\lambda_1(A)}{\lambda_n(A)}$ is the conditioning number of matrix A , $\lambda_1(A) \geq \dots \geq \lambda_n(A)$ are the eigenvalues of matrix A

Note: Compare the coefficient of the geometric progression with its analog in gradient descent.

Numerical results

$$f(x) = \frac{1}{2}x^T Ax - b^T x \rightarrow \min_{x \in \mathbb{R}^n}$$

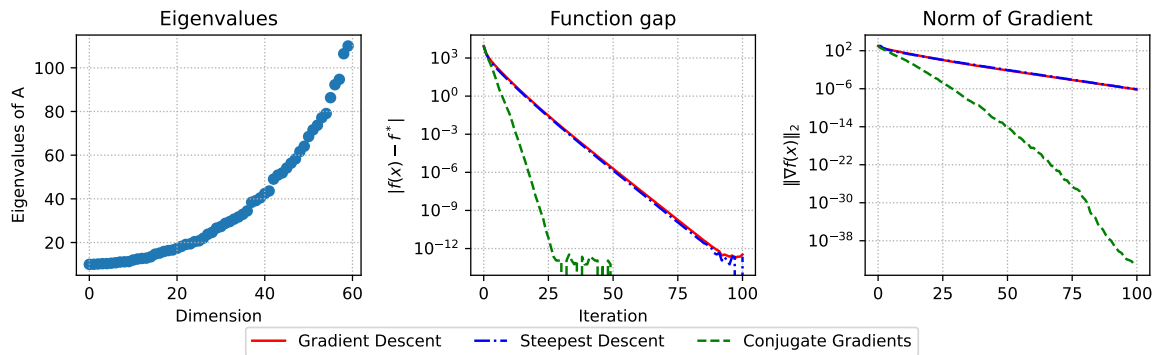
Convex quadratics. $n=60$, random matrix.



Numerical results

$$f(x) = \frac{1}{2}x^T A x - b^T x \rightarrow \min_{x \in \mathbb{R}^n}$$

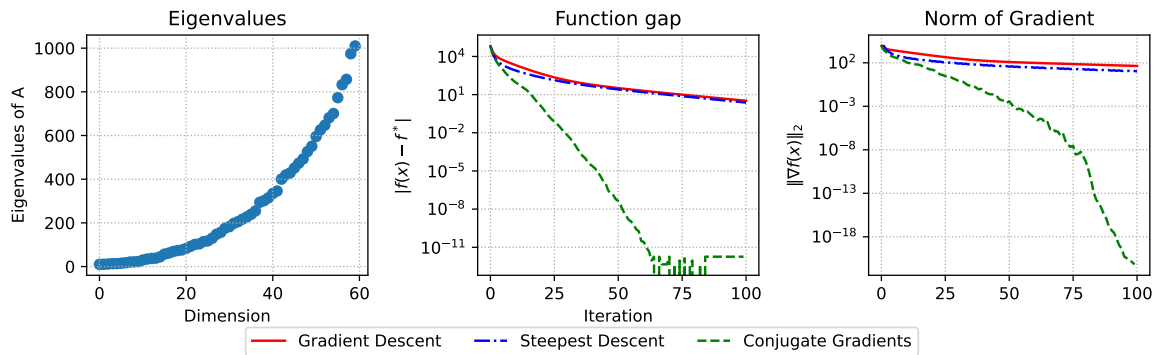
Strongly convex quadratics. $n=60$, random matrix.



Numerical results

$$f(x) = \frac{1}{2}x^T Ax - b^T x \rightarrow \min_{x \in \mathbb{R}^n}$$

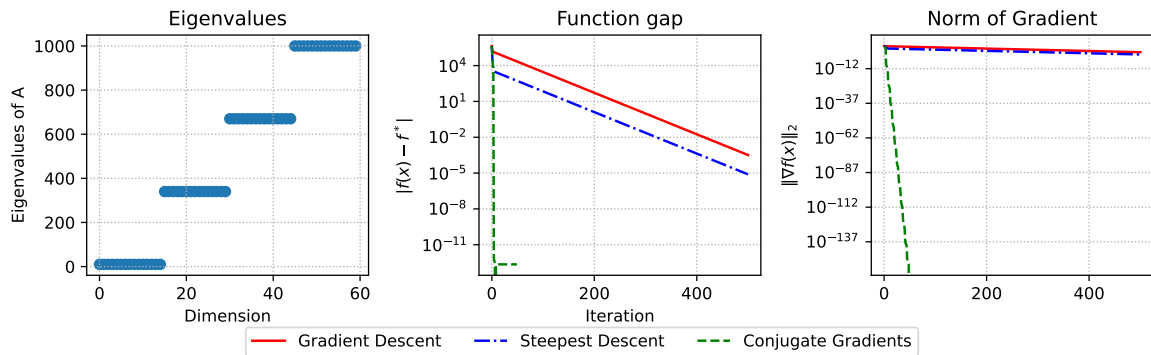
Strongly convex quadratics. $n=60$, random matrix.



Numerical results

$$f(x) = \frac{1}{2}x^T Ax - b^T x \rightarrow \min_{x \in \mathbb{R}^n}$$

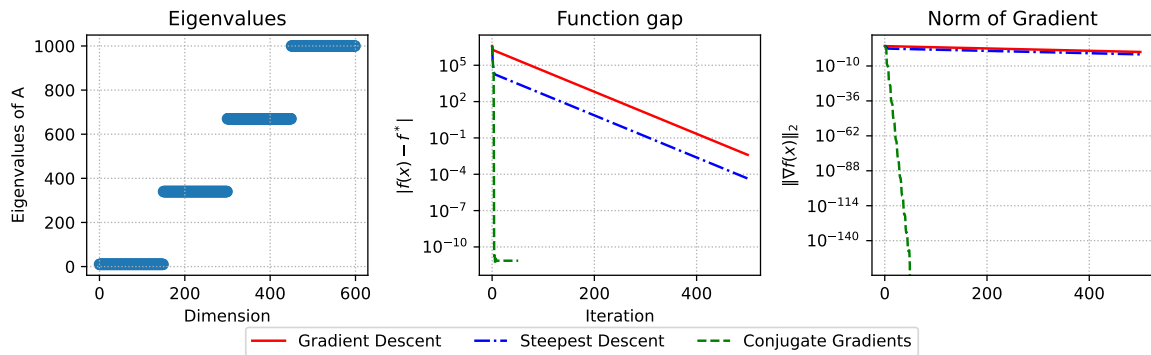
Strongly convex quadratics. $n=60$, clustered matrix.



Numerical results

$$f(x) = \frac{1}{2}x^T A x - b^T x \rightarrow \min_{x \in \mathbb{R}^n}$$

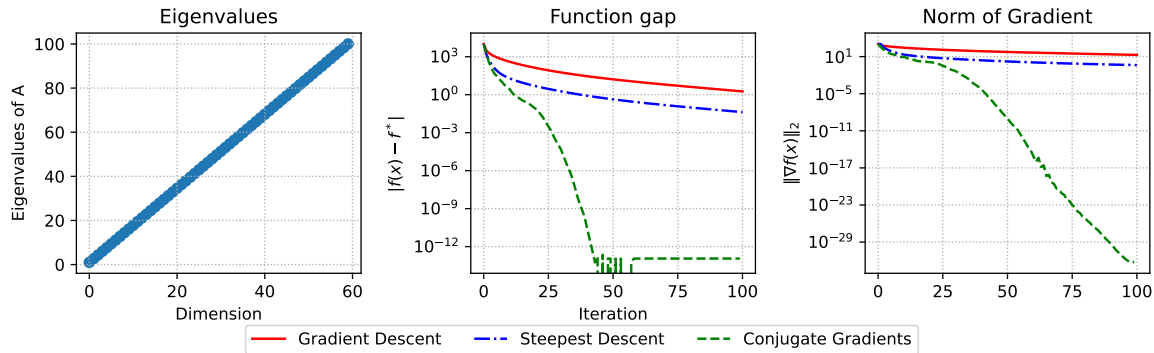
Strongly convex quadratics. $n=600$, clustered matrix.



Numerical results

$$f(x) = \frac{1}{2}x^T A x - b^T x \rightarrow \min_{x \in \mathbb{R}^n}$$

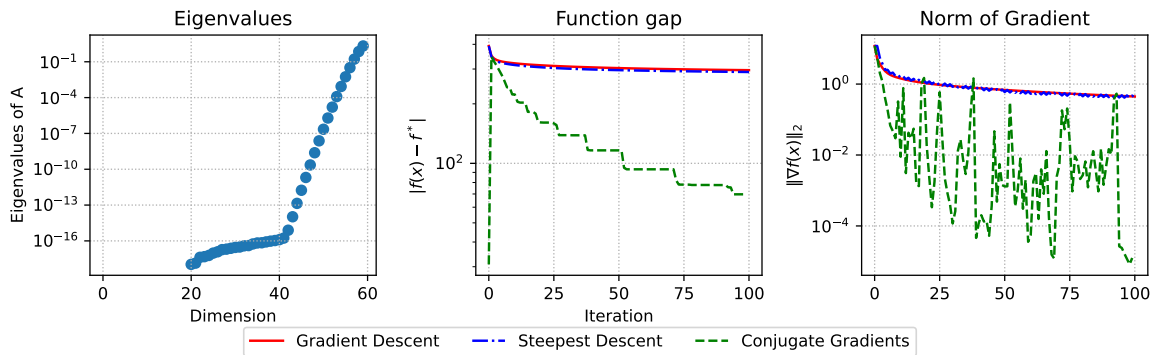
Strongly convex quadratics. $n=60$, uniform spectrum matrix.



Numerical results

$$f(x) = \frac{1}{2}x^T A x - b^T x \rightarrow \min_{x \in \mathbb{R}^n}$$

Strongly convex quadratics. $n=60$, Hilbert matrix.



Non-linear conjugate gradient method

In case we do not have an analytic expression for a function or its gradient, we will most likely not be able to solve the one-dimensional minimization problem analytically. Therefore, step 2 of the algorithm is replaced by the usual line search procedure. But there is the following mathematical trick for the fourth point:

For two iterations, it is fair:

$$x_{k+1} - x_k = cd_k,$$

where c is some kind of constant. Then for the quadratic case, we have:

$$\nabla f(x_{k+1}) - \nabla f(x_k) = (Ax_{k+1} - b) - (Ax_k - b) = A(x_{k+1} - x_k) = cAd_k$$

Expressing from this equation the work $Ad_k = \frac{1}{c} (\nabla f(x_{k+1}) - \nabla f(x_k))$, we get rid of the “knowledge” of the function in step definition β_k , then point 4 will be rewritten as:

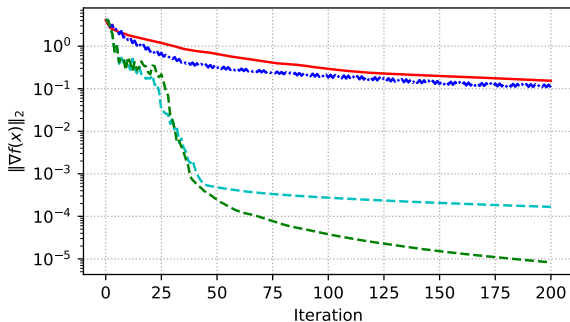
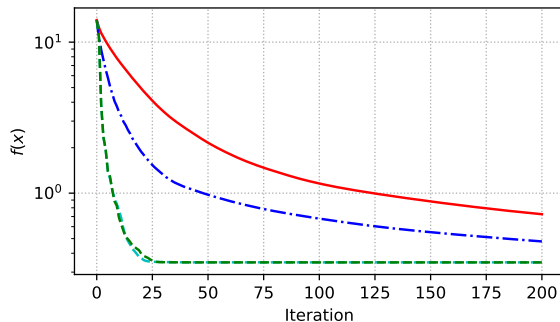
$$\beta_k = \frac{\nabla f(x_{k+1})^\top (\nabla f(x_{k+1}) - \nabla f(x_k))}{d_k^\top (\nabla f(x_{k+1}) - \nabla f(x_k))}.$$

This method is called the Polack-Ribier method.

Numerical results

$$f(x) = \frac{\mu}{2} \|x\|_2^2 + \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-y_i \langle a_i, x \rangle)) \rightarrow \min_{x \in \mathbb{R}^n}$$

Regularized binary logistic regression. $n=300$. $m=1000$. $\mu=0$

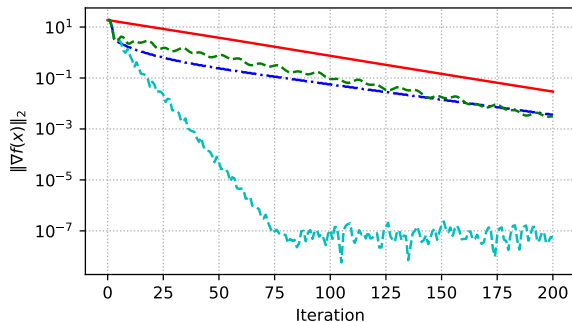
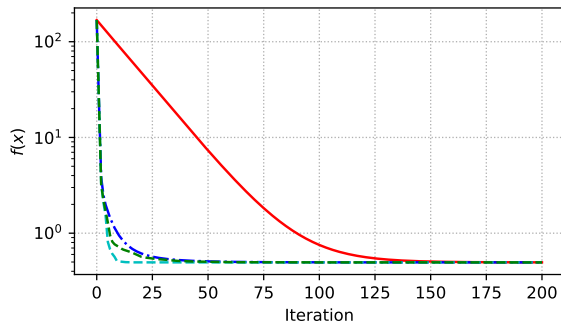


— Gradient Descent -.- Steepest Descent - - - Conjugate Gradients PR - - - Conjugate Gradients FR

Numerical results

$$f(x) = \frac{\mu}{2} \|x\|_2^2 + \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-y_i \langle a_i, x \rangle)) \rightarrow \min_{x \in \mathbb{R}^n}$$

Regularized binary logistic regression. $n=300$. $m=1000$. $\mu=1$

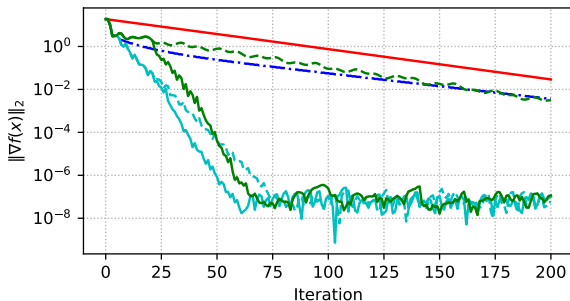
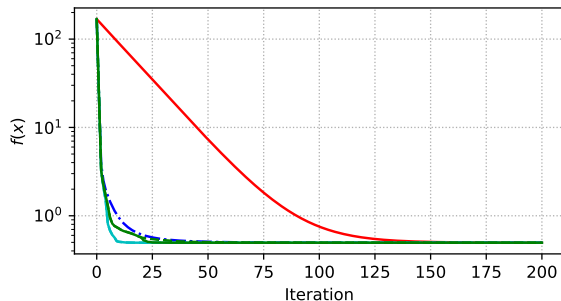


— Gradient Descent -.- Steepest Descent - - - Conjugate Gradients PR - - - Conjugate Gradients FR

Numerical results

$$f(x) = \frac{\mu}{2} \|x\|_2^2 + \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-y_i \langle a_i, x \rangle)) \rightarrow \min_{x \in \mathbb{R}^n}$$

Regularized binary logistic regression. $n=300$. $m=1000$. $\mu=1$

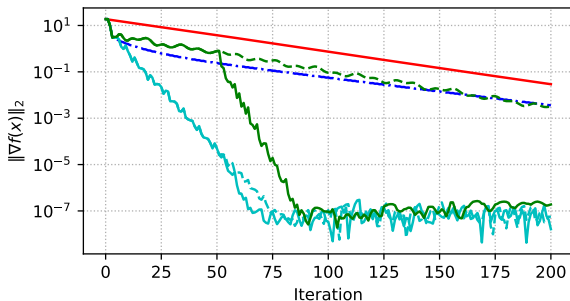
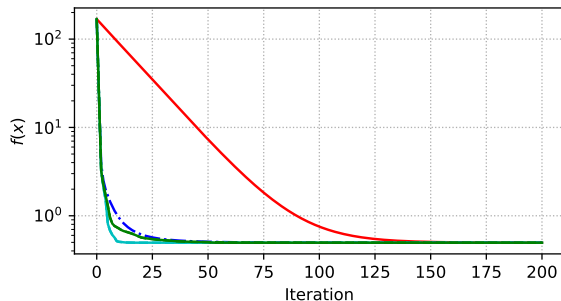


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|------------------------|--------------------------------------|--------------------------------------|
| — Gradient Descent | - - - Conjugate Gradients PR | - - - Conjugate Gradients FR |
| - . - Steepest Descent | — Conjugate Gradients PR. restart 20 | — Conjugate Gradients FR. restart 20 |

Numerical results

$$f(x) = \frac{\mu}{2} \|x\|_2^2 + \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-y_i \langle a_i, x \rangle)) \rightarrow \min_{x \in \mathbb{R}^n}$$

Regularized binary logistic regression. $n=300$. $m=1000$. $\mu=1$

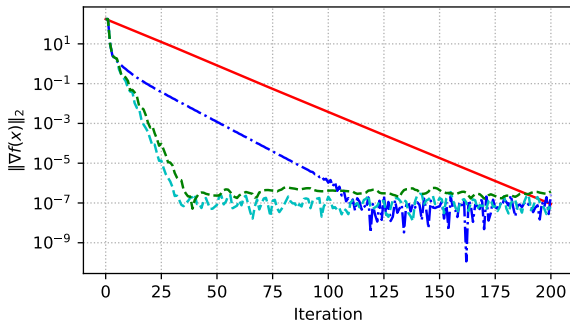
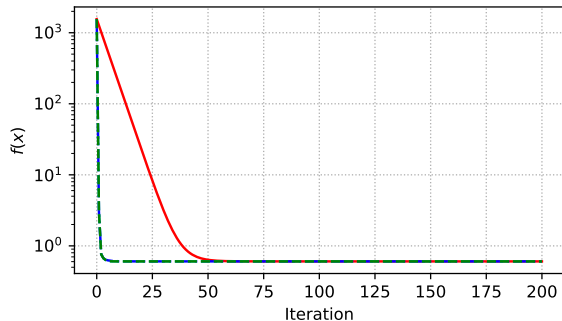


- | | | |
|------------------------|--------------------------------------|--------------------------------------|
| — Gradient Descent | - - - Conjugate Gradients PR | - - - Conjugate Gradients FR |
| - . - Steepest Descent | — Conjugate Gradients PR. restart 50 | — Conjugate Gradients FR. restart 50 |

Numerical results

$$f(x) = \frac{\mu}{2} \|x\|_2^2 + \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-y_i \langle a_i, x \rangle)) \rightarrow \min_{x \in \mathbb{R}^n}$$

Regularized binary logistic regression. $n=300$. $m=1000$. $\mu=10$

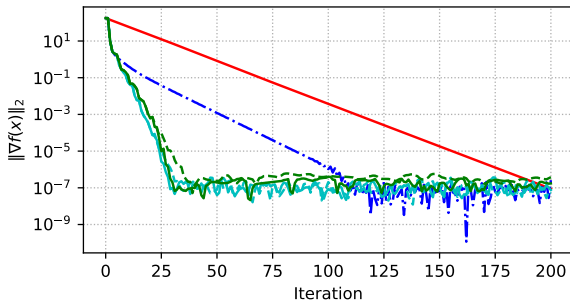
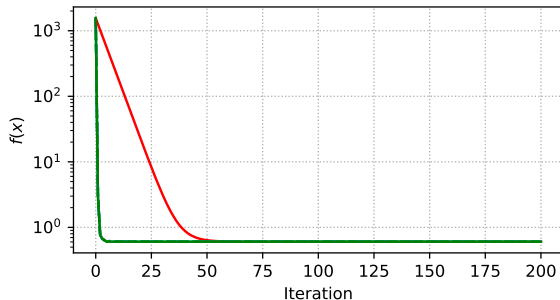


— Gradient Descent -.- Steepest Descent - - - Conjugate Gradients PR - - - Conjugate Gradients FR

Numerical results

$$f(x) = \frac{\mu}{2} \|x\|_2^2 + \frac{1}{m} \sum_{i=1}^m \log(1 + \exp(-y_i \langle a_i, x \rangle)) \rightarrow \min_{x \in \mathbb{R}^n}$$

Regularized binary logistic regression. $n=300$. $m=1000$. $\mu=10$



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|--|--|---|
| — Gradient Descent | - - - Conjugate Gradients PR | - - - Conjugate Gradients FR |
| - · - Steepest Descent | — Conjugate Gradients PR. restart 20 | — Conjugate Gradients FR. restart 20 |