

# Conjugate gradients method

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## Strongly convex quadratics

Consider the following quadratic optimization problem:

Optimality conditions

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

$$Ax^* = b$$

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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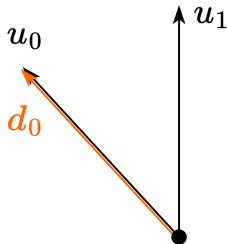


Figure 4: Illustration of Gram-Schmidt orthogonalization process



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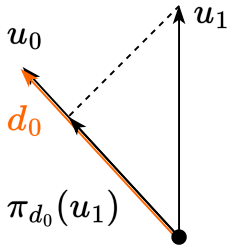


Figure 5: Illustration of Gram-Schmidt orthogonalization process

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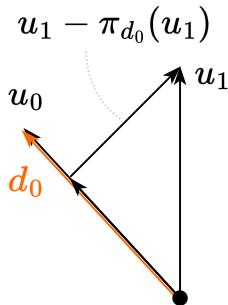


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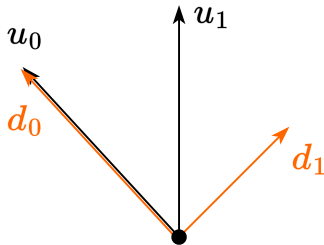
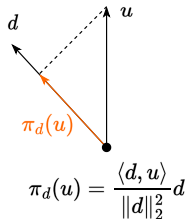


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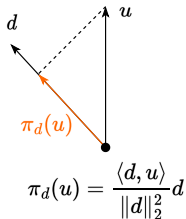
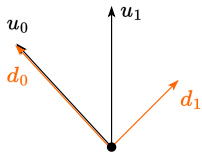


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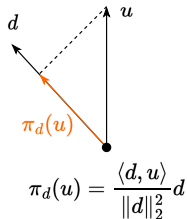
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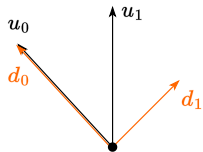


$$\pi_d(u) = \frac{\langle d, u \rangle}{\|d\|_2^2} d$$

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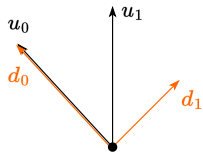




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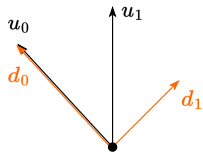
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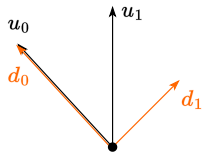
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$$d_k = u_k + \sum_{i=0}^{k-1} \beta_{ik} d_i \quad \beta_{ik} = -\frac{\langle d_i, u_k \rangle}{\langle d_i, d_i \rangle} \quad (2)$$

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

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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

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If a set of vectors  $d_1, \dots, d_n$  - are  $A$ -conjugate (each pair of vectors is  $A$ -conjugate), these vectors are linearly independent.  $A \in \mathbb{S}_{++}^n$ .

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Multiply by  $d_j^T A$ .

$$= d_j^T A \left( \sum_{i=1}^n \alpha_i d_i \right)$$



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If a set of vectors  $d_1, \dots, d_n$  - are  $A$ -conjugate (each pair of vectors is  $A$ -conjugate), these vectors are linearly independent.  $A \in \mathbb{S}_{++}^n$ .

## Proof

We'll show, that if  $\sum_{i=1}^n \alpha_i d_i = 0$ , than all coefficients should be equal to zero:

$$0 = \sum_{i=1}^n \alpha_i d_i$$

Multiply by  $d_j^T A$ .

$$= d_j^T A \left( \sum_{i=1}^n \alpha_i d_i \right) = \sum_{i=1}^n \alpha_i d_j^T A d_i$$

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Thus,  $\alpha_j = 0$ , for all other indices one has to perform the same process

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

$$e_{k+1} = e_0 + \sum_{i=1}^k \alpha_i d_i. \quad (5)$$



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Consider residual of the CD method at  $k$  iteration  $r_k$ , then for any  $i < k$ :

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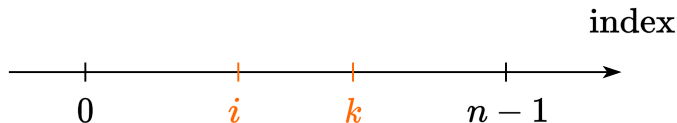
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Multiply both sides by  $-d_i^T A$ .

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



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

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All residuals are pairwise orthogonal to each other in the CG method:

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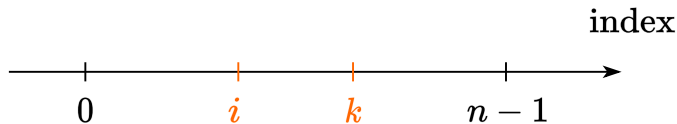
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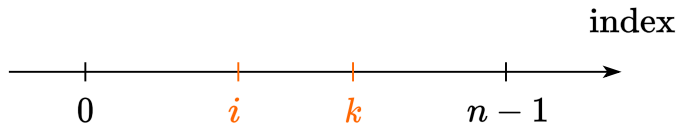
$$r_k^T d_i = r_k^T u_i + \sum_{j=0}^{k-1} \beta_{ji} r_k^T d_j$$

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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Lemma 6. Residual recalculation

$$r_{k+1} = r_k - \alpha_k A d_k \quad (12)$$

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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

Consider the Gram-Schmidt process in the CG method

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



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## Gram-Schmidt process in CG method

Consider the Gram-Schmidt process in the CG method

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

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

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

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.  $n=60$ , 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.  $n=60$ , 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

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

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  $\beta_k$ , then point 4 will be rewritten as:

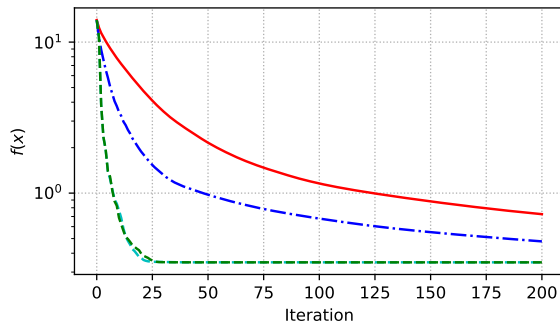
$$\beta_k = \frac{\nabla f(x_{k+1})^\top (\nabla f(x_{k+1}) - \nabla f(x_k))}{d_k^\top (\nabla f(x_{k+1}) - \nabla f(x_k))}.$$

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.  $n=300$ .  $m=1000$ .  $\mu=0$

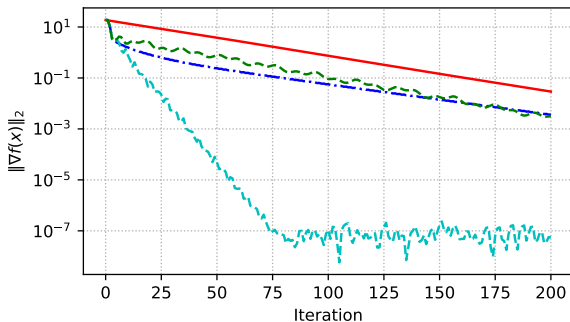


— Gradient Descent    -.- Steepest Descent    - - - Conjugate Gradients PR    - - - Conjugate Gradients FR

## 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.  $n=300$ .  $m=1000$ .  $\mu=1$



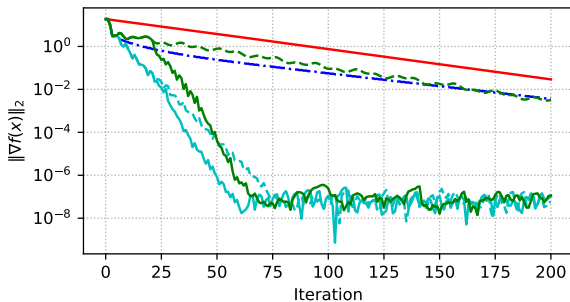
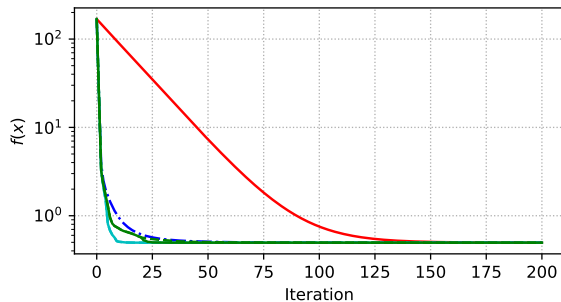
— Gradient Descent    -.- Steepest Descent    - - - Conjugate Gradients PR    - - - Conjugate Gradients FR



# Numerical results

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

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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.  $n=300$ .  $m=1000$ .  $\mu=1$

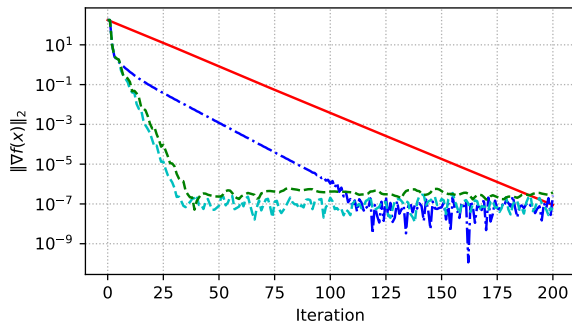
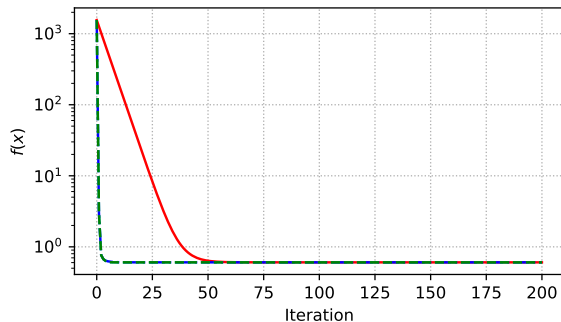


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|------------------------|--------------------------------------|--------------------------------------|
| — Gradient Descent     | - - - Conjugate Gradients PR         | - - - Conjugate Gradients FR         |
| - . - Steepest Descent | — Conjugate 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.  $n=300$ .  $m=1000$ .  $\mu=10$

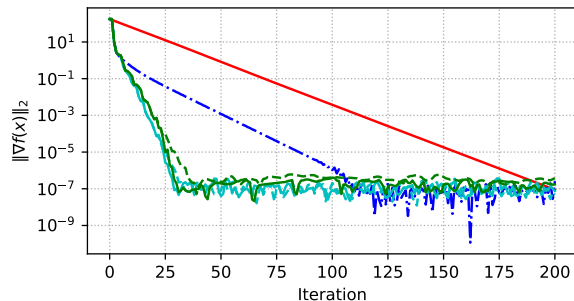
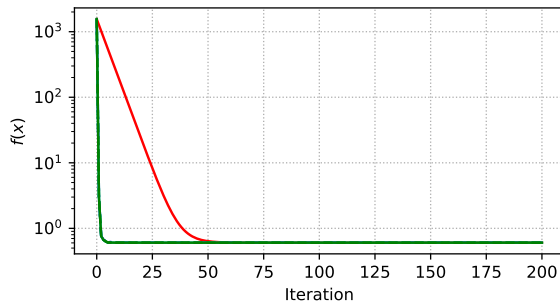


— Gradient Descent    -.- Steepest Descent    - - - Conjugate Gradients PR    - - - Conjugate Gradients FR

# 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.  $n=300$ .  $m=1000$ .  $\mu=10$



- |  |  |   |
|--|--|---|
| <span style="color: red;">—</span> Gradient Descent      | <span style="color: cyan;">- - -</span> Conjugate Gradients PR         | <span style="color: green;">- - -</span> Conjugate Gradients FR         |
| <span style="color: blue;">- . -</span> Steepest Descent | <span style="color: cyan;">—</span> Conjugate Gradients PR. restart 20 | <span style="color: green;">—</span> Conjugate Gradients FR. restart 20 |