Conjugate gradients method

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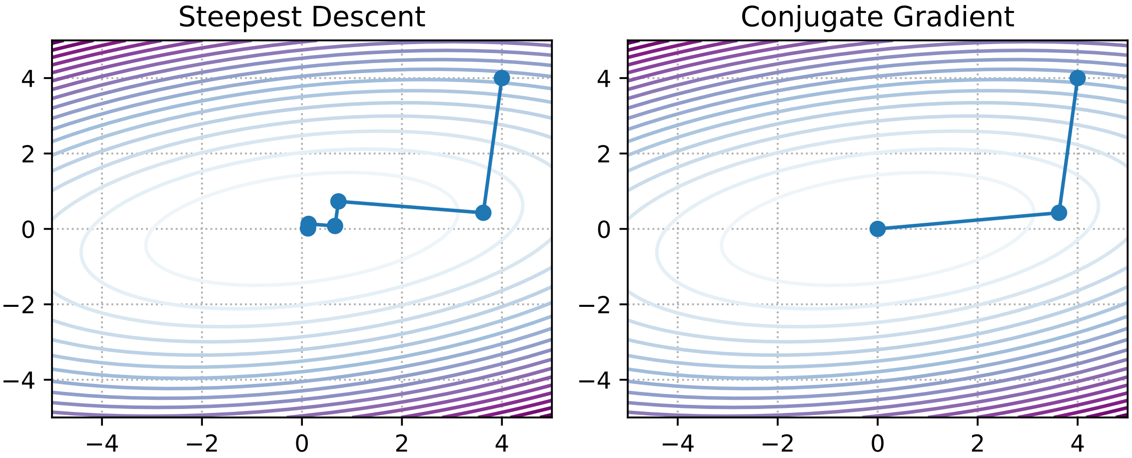
Strongly convex quadratics

Consider the following quadratic optimization problem:

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

Optimality conditions

$$\boxed{Ax^* = b}$$



Exact line search aka steepest descent

$x_{k+1} = x_k - \alpha_k \nabla f(x_k)$

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

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:

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

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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:

$\nabla f(x_{k+1}) = Ax_{k+1} =$

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

grad $f(x)$

Optimality conditions:

$\nabla f = Ax$

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

Optimal value for quadratics

$$\nabla f(x_k)^\top A(x_k - \alpha \nabla f(x_k)) - \nabla f(x_k)^\top b = 0$$

$$\boxed{\alpha_k = \frac{\nabla f(x_k)^T \nabla f(x_k)}{\nabla f(x_k)^T A \nabla f(x_k)}}$$

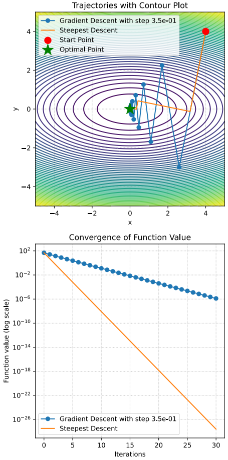


Figure 1: Steepest Descent

Open In Colab ♣

Conjugate directions. A-orthogonality.

идеальный мир $b \neq 0$ реальный мир

$A = I$ $A \neq I$

v_1 and v_2 are orthogonal

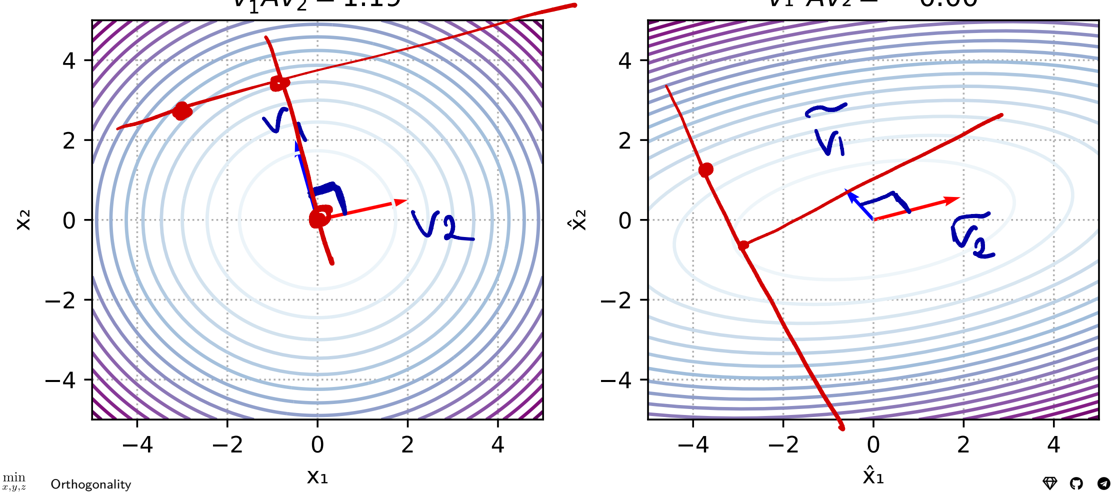
$v_1^T v_2 = 0.00$

$v_1^T A v_2 = 1.19$

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

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

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



Conjugate directions. A-orthogonality.

Suppose, we have two coordinate systems and some quadratic function $f(x) = \frac{1}{2}x^T I x$ 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 $A \in \mathbb{S}^n_{++}$.

$$f(x) = \frac{1}{2}x^T I x \qquad\qquad f(\hat{x}) = \frac{1}{2}\hat{x}^T A \hat{x}$$

Since $\boxed{A = Q\Lambda Q^T:}$

$$\frac{1}{2}\hat{x}^T A \hat{x}$$

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$$\frac{1}{2}x^T I x \qquad\qquad \frac{1}{2}\hat{x}^T A \hat{x}$$

$\Lambda = \text{diag}(\lambda_1 \ldots \lambda_n)$

$\Lambda^{\frac{1}{2}} = \text{diag}(\sqrt{\lambda_1} \ldots \sqrt{\lambda_n})$

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

$$\frac{1}{2}\hat{x}^T A \hat{x} = \frac{1}{2}\hat{x}^T Q\Lambda Q^T \hat{x} = \frac{1}{2}\hat{x}^T Q\Lambda^{\frac{1}{2}}\Lambda^{\frac{1}{2}} Q^T \hat{x}$$

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из реального

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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

$$\boxed{x^T A y = 0} \qquad \Leftrightarrow \qquad x \perp_A y$$

When $A = I$, A-orthogonality becomes orthogonality. $A = I \Rightarrow x \perp y$

Gram–Schmidt process

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

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

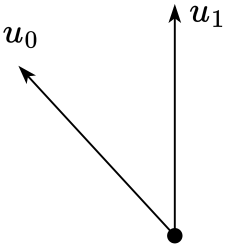

Figure 3: Illustration of Gram-Schmidt orthogonalization process

Gram–Schmidt process

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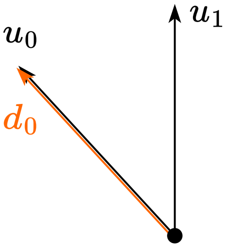

Figure 4: Illustration of Gram-Schmidt orthogonalization process

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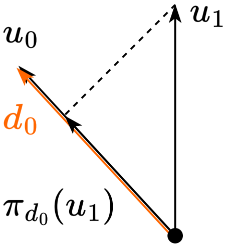

проекция u_1 на d_0

Figure 5: Illustration of Gram-Schmidt orthogonalization process

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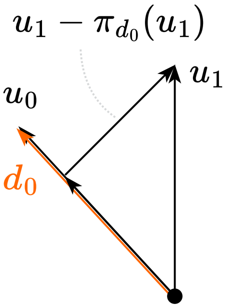

Figure 6: Illustration of Gram-Schmidt orthogonalization process

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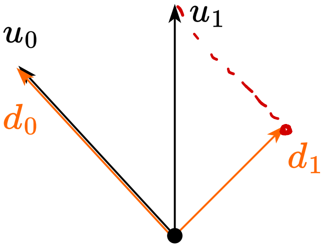
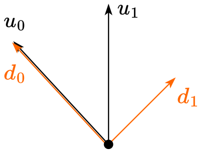
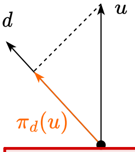


Figure 7: Illustration of Gram-Schmidt orthogonalization process

Gram–Schmidt process

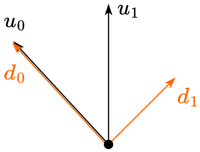
Input: n linearly independent vectors $u_0, \ldots, u_{n-1}$.





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

Gram–Schmidt process



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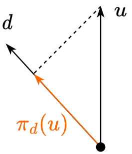
$$d_0 = u_0$$



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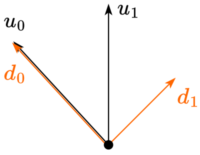
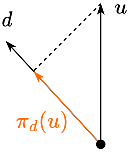
Gram–Schmidt process





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$$d_0 = u_0$$
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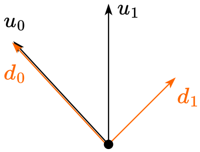
Gram–Schmidt process



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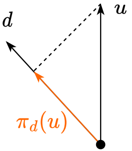

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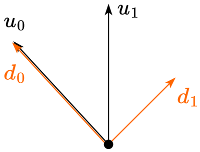

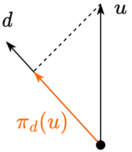

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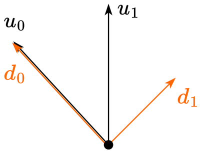

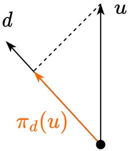

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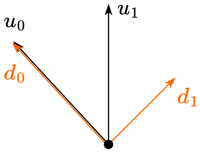
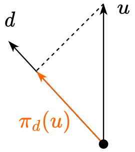
Gram–Schmidt process





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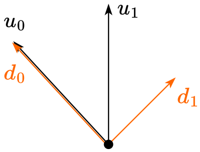

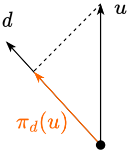

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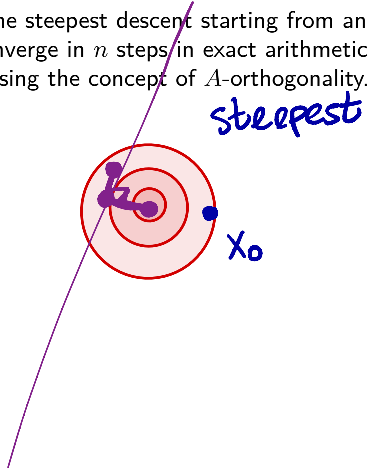
\end{aligned}$$

$$\boxed{d_k = u_k + \sum_{i=0}^{k-1} \beta_{ik} d_i} \qquad \beta_{ik} = -\frac{\langle d_i, u_k\rangle}{\langle d_i, d_i\rangle} \tag{2}$$

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 would like to build a method, that goes from x_0 to the x^* for the quadratic problem with stepsizes α_i, which is, in fact, just the decomposition of $x^* - x_0$ to some basis:

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

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- We would like to build a method, that goes from x_0 to the x^* for the quadratic problem with stepsizes α_i, which is, in fact, just the decomposition of $x^* - x_0$ to some basis:

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

- 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

метод сопряженных направлений.

Thus, we formulate an algorithm:

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

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Thus, we formulate an algorithm:

1. Let $k = 0$ and $x_k = x_0$, count $d_k = d_0 = -\nabla f(x_0)$.
2. By the procedure of line search we find the optimal length of step. Calculate α minimizing $f(x_k + \alpha_k d_k)$ by the formula

$$\boxed{\alpha_k = -\frac{d_k^\top (Ax_k - b)}{d_k^\top A d_k}} \tag{3}$$

наиск. спуск в направлении d_k из точки x_k

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$$\left(-\nabla f(x_{k+1}) + \beta_k d_k\right)^\top A d_k = 0$$

$$\Rightarrow \beta_k = \ldots$$

Idea of Conjugate Directions (CD) method

Сх-ть за $\leq n$ шагов

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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

Lemma 1. Linear independence of A-conjugate vectors.

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

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Proof предполагаем противное

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выбираем индекс J

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$$= \alpha_j d_j^\top A d_j + 0 + \ldots + 0$$

в силу A-орт.

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\begin{aligned}
0 &= \sum_{i=1}^n \alpha_i d_i \\
\text{Multiply by } d_j^T A \cdot \qquad &= d_j^\top A \left(\sum_{i=1}^n \alpha_i d_i \right) = \sum_{i=1}^n \alpha_i d_j^\top A d_i \\
&= \alpha_j d_j^\top A d_j + 0 + \ldots + 0
\end{aligned}
$$

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

Proof of convergence

We will introduce the following notation:

- $\boxed{r_k = b - Ax_k}$ - residual,

$r = -\nabla f$

Proof of convergence

$Ax^* = b$

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$$r_k = -Ae_k. \tag{4}$$

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

$$\boxed{e_{k+1} = e_0 + \sum_{i=1}^{k} \alpha_i d_i.} \tag{5}$$

Proof of convergence

Lemma 2. Convergence of conjugate direction method.

Suppose, we solve n-dimensional quadratic convex optimization problem (1). The conjugate directions method

$$x_{k+1} = x_0 + \sum_{i=0}^{k} \alpha_i d_i$$

with $\alpha_i = \frac{\langle d_i, r_i \rangle}{\langle d_i, A d_i \rangle}$ taken from the line search, converges for at most n steps of the algorithm.

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with $\alpha_i = \frac{\langle d_i, r_i \rangle}{\langle d_i, Ad_i \rangle}$ taken from the line search, converges for at most n steps of the algorithm.

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

Proof

1. We need to prove, that $\delta_i = -\alpha_i$:

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$$d_k^T A \left(e_0 + \sum_{i=0}^{k-1} \alpha_i d_i \right)$$

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$$
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$$
\delta_k = \frac{d_k^T A e_k}{d_k^T A d_k} = -\frac{d_k^T r_k}{d_k^T A d_k} \Leftrightarrow \delta_k = -\alpha_k
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Lemms for convergence

Lemma 3. Error decomposition

$$e_i = \sum_{j=i}^{n-1} -\alpha_j d_j \tag{6}$$

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$$x_i = x_0 + \sum_{j=0}^{i-1} \alpha_j d_j$$

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Lemma 4. Residual is orthogonal to all previous directions for CD

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

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Proof

Let's write down (6) for some fixed index k:

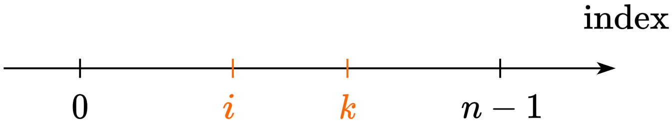
$$e_k = \sum_{j=k}^{n-1} -\alpha_j d_j$$

$i<k$

Multiply both sides by $-d_i^T A \cdot$

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

$r_k^T d_i = 0$



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

The idea of the Conjugate Gradients (CG) method

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

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$$\langle x, y \rangle \rightarrow \langle x, y \rangle_A$$

$$\langle x, y \rangle_A = x^T A y$$

The idea of the Conjugate Gradients (CG) method

$r_0 = -\nabla f_0$

$b - Ax_0$

$r_k = -\nabla f(x_k)$

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- The main idea is that for an arbitrary CD method, the Gramm-Schmidt process is quite computationally expensive and requires a quadratic number of vector addition and scalar product operations $\mathcal{O}\left(n^2\right)$, while in the case of CG, we will show that the complexity of this procedure can be reduced to linear $\mathcal{O}\left(n\right)$.

The idea of the Conjugate Gradients (CG) method

- It is literally the Conjugate Direction method, where we have a special (effective) choice of $d_0, \ldots, d_{n-1}$.
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$$\text{CG} = \text{CD} + r_0, \ldots, r_{n-1} \text{ as starting vectors for Gram–Schmidt} + A\text{-orthogonality.}$$

Lemms for convergence

Lemma 5. Residuals are orthogonal to each other in the CG method

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

$$r_i^T r_k = 0 \qquad \forall i \neq k \tag{8}$$

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Выход Вход

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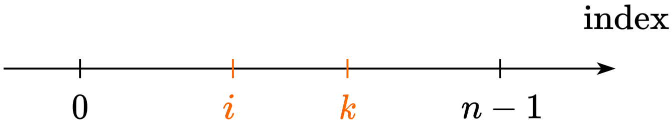

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Multiply both sides of (9) by $r_k^T \cdot$ for some index k:

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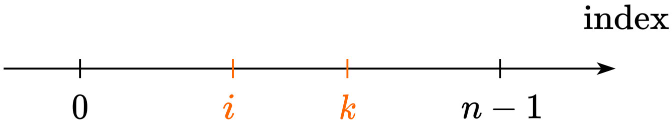

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пусть $i < k$

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

$j < k$

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:

$\boxed{r_k^T u_i = 0}$ for CD $\boxed{r_k^T r_i = 0 \text{ for CG}}$ $i < k$

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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CG: $\boxed{r_k^T d_k = r_k^T u_k}$

Lemma 6. Residual recalculation

$$\boxed{r_{k+1} = r_k - \alpha_k A d_k} \tag{12}$$

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$$
\boxed{r_{k+1} = -Ae_{k+1}} = -A\left(e_k + \alpha_k d_k\right) = \underline{-Ae_k} - \alpha_k A d_k = \underline{r_k} - \alpha_k A d_k
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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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$u_i = r_i \leftarrow$ CG

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$$r_i^T A d_j = \frac{1}{\alpha_j} \left[\langle r_i, r_j \rangle - \langle r_i, r_{j+1} \rangle \right]$$

Gram-Schmidt process in CG method

$r_i^T r_k = 0$

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$j = i - 1$

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Gram-Schmidt process in CG method

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

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 $i = j + 1$:

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

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And for the direction

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

Conjugate gradients method

$\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$ $\quad -\nabla f(x_0)$

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

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

$k := 0$

GS + A

repeat

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

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

шаг вдоль d_k с наилучш. α

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

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

$\sim(n^2)$

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

в общем CD $+\beta_{k-1} d_{k-1} + \beta_{k-2} d_{k-2}$

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

построение нового A-сопр. напр.

$k := k + 1$

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

ускоренная лин. сх-ть

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

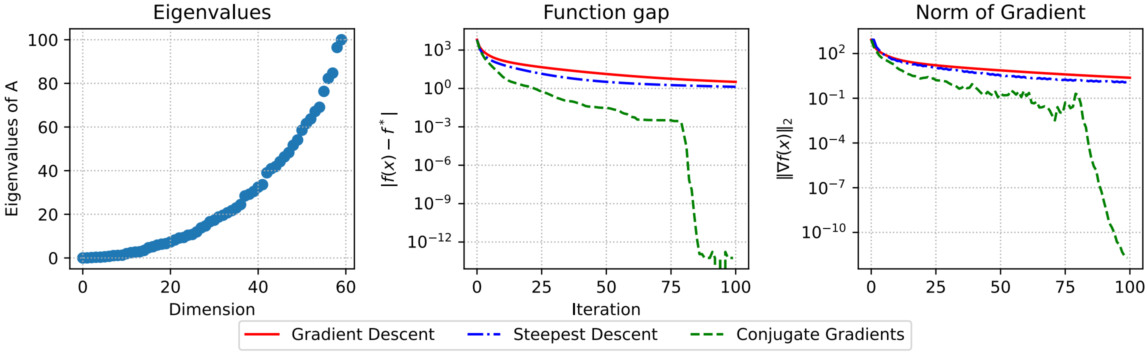
where $\|x\|_A^2 = x^\top A x$ and $\kappa(A) = \frac{\lambda_1(A)}{\lambda_n(A)}$ is the conditioning number of matrix A, $\lambda_1(A) \geq ... \geq \lambda_n(A)$ are the eigenvalues of matrix A

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

Numerical results

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

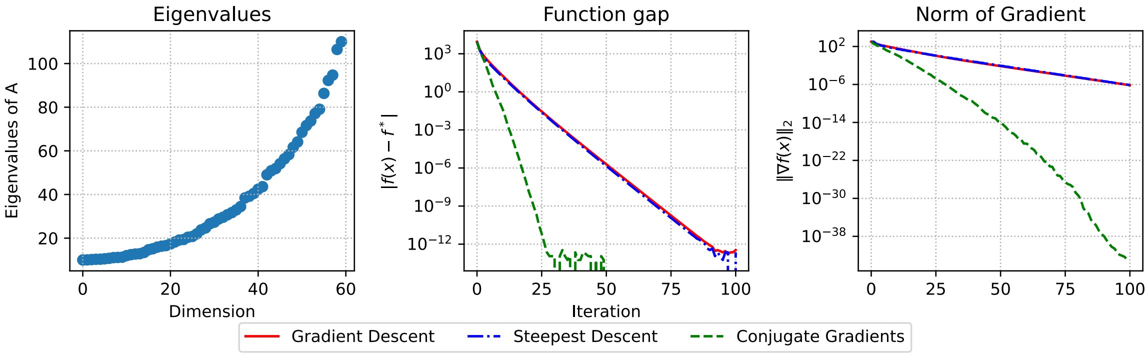
Convex quadratics. n=60, random matrix.



Numerical results

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

Strongly convex quadratics. n=60, random matrix.



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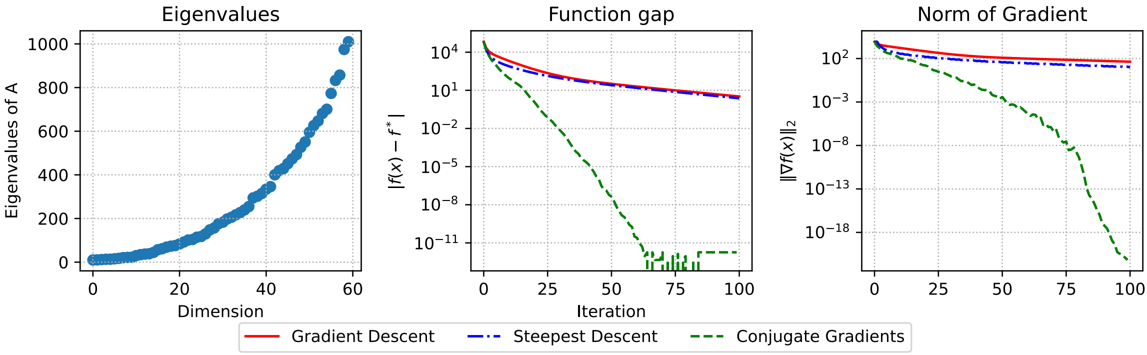
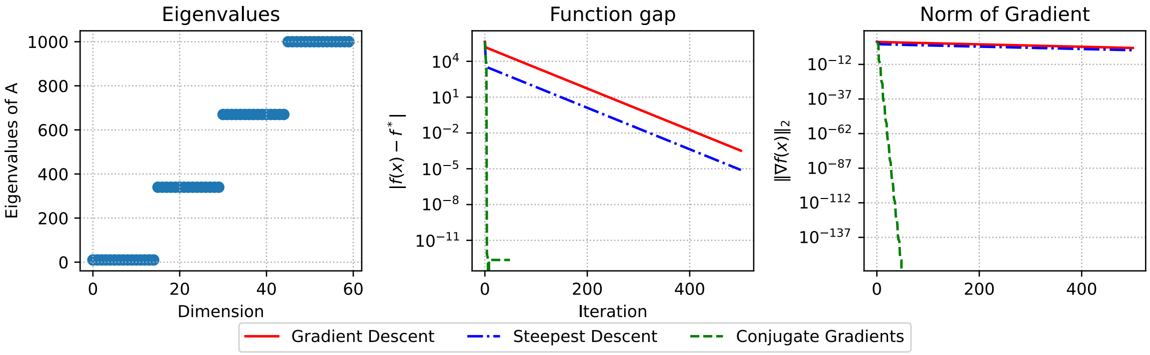


Numerical results

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

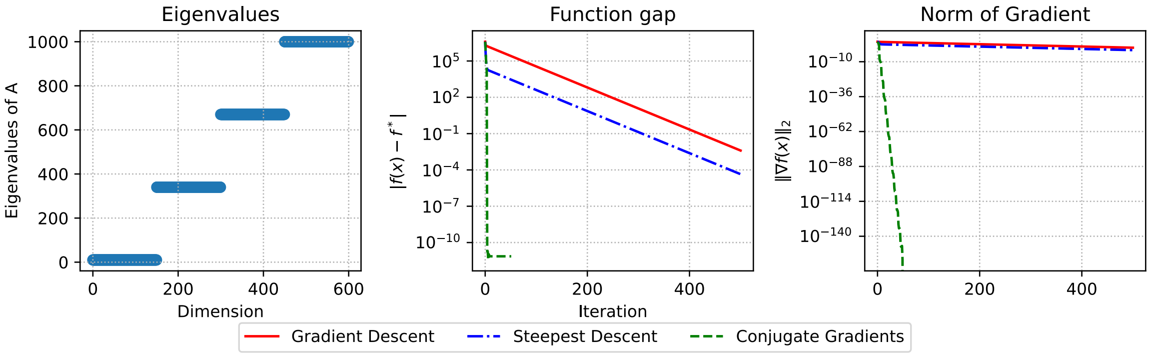
Strongly convex quadratics. n=60, clustered matrix.



Numerical results

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

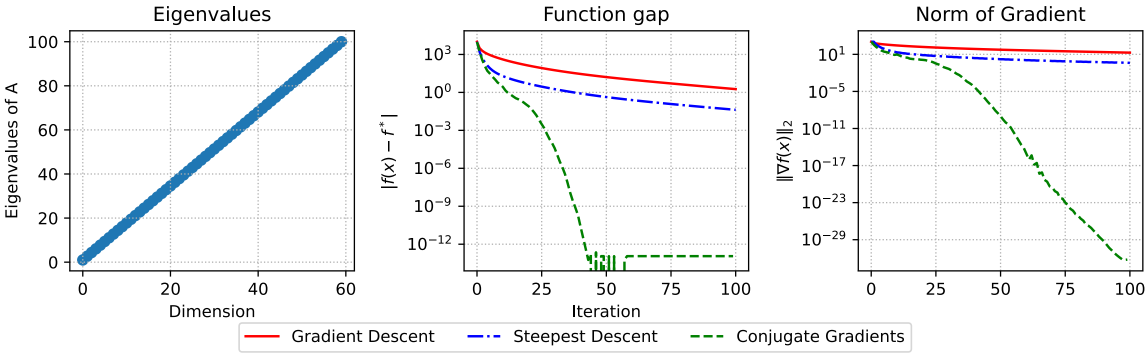
Strongly convex quadratics. n=600, clustered matrix.



Numerical results

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

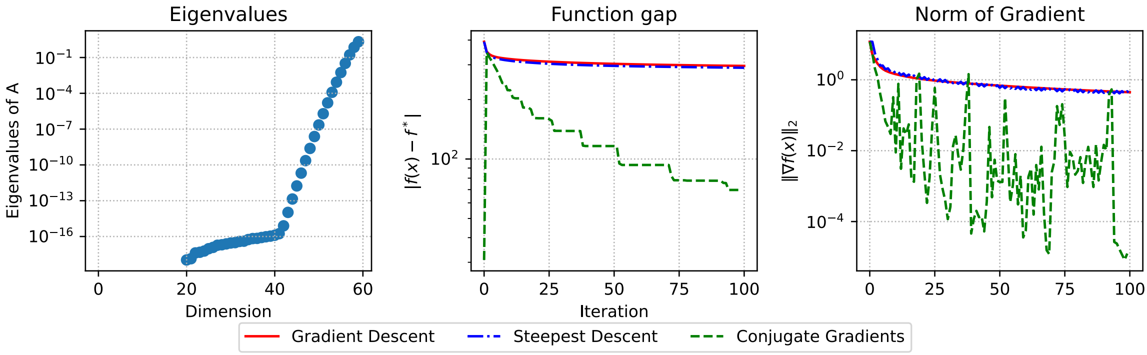
Strongly convex quadratics. n=60, uniform spectrum matrix.



Numerical results

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

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 $Ad_k = \dfrac{1}{c}\left(\nabla f(x_{k+1}) - \nabla f(x_k)\right)$, we get rid of the "knowledge" of the function in step definition β_k, then point 4 will be rewritten as:

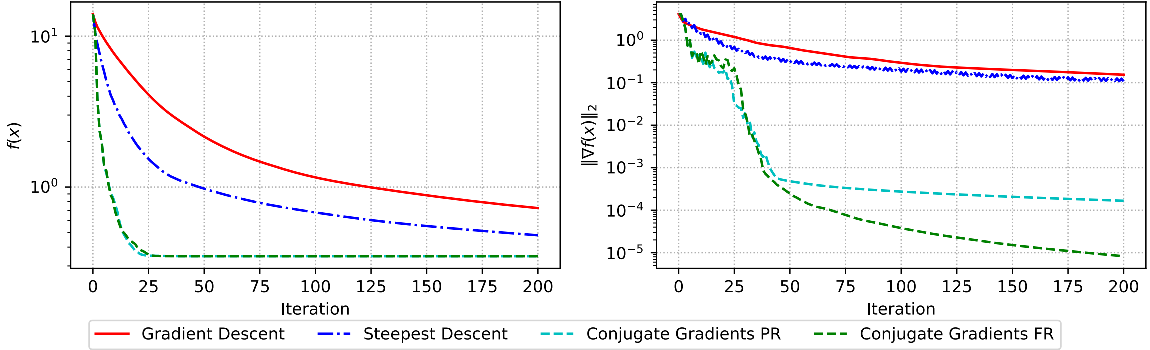
$$\beta_k = \frac{\nabla f(x_{k+1})^\top (\nabla f(x_{k+1}) - \nabla f(x_k))}{d_k^\top (\nabla f(x_{k+1}) - \nabla f(x_k))}.$$

This method is called the Polack-Ribier method.

Numerical results

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

Regularized binary logistic regression. n=300. m=1000. μ=0



Numerical results

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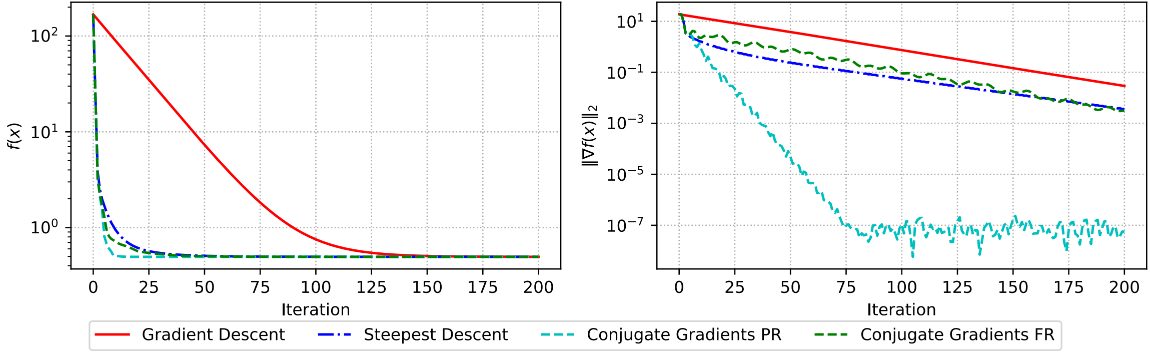
Regularized binary logistic regression. n=300. m=1000. μ=1



Numerical results

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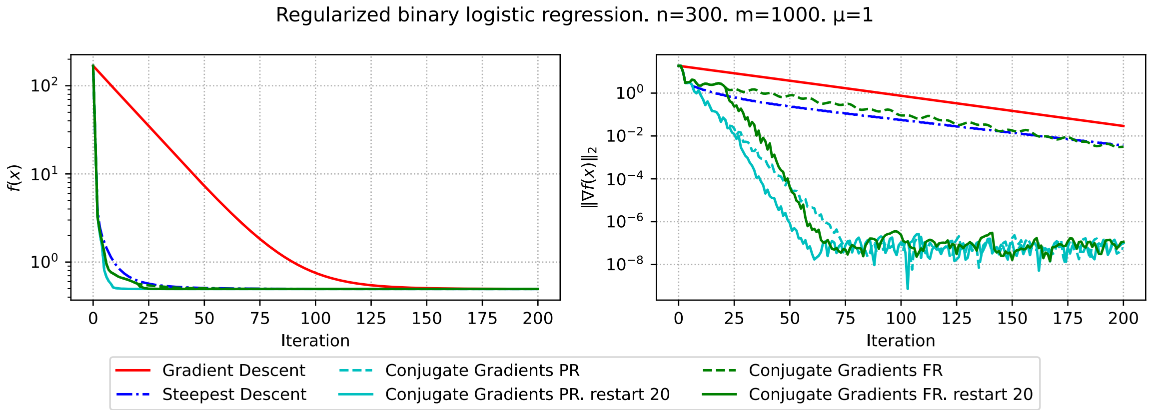
f(x) = \frac{\mu}{2}\|x\|_2^2 + \frac{1}{m}\sum_{i=1}^{m} \log(1 + \exp(-y_i\langle a_i, x\rangle)) \to \min_{x\in\mathbb{R}^n}
$$



Numerical results

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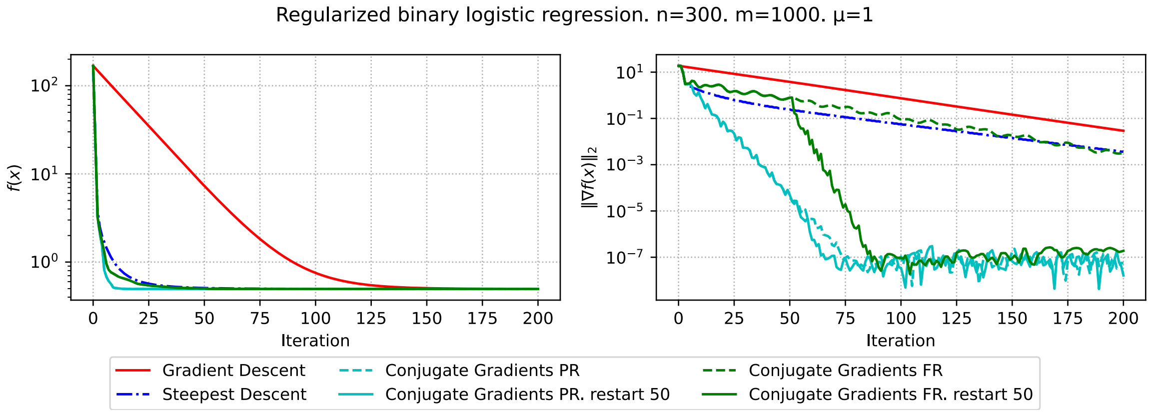

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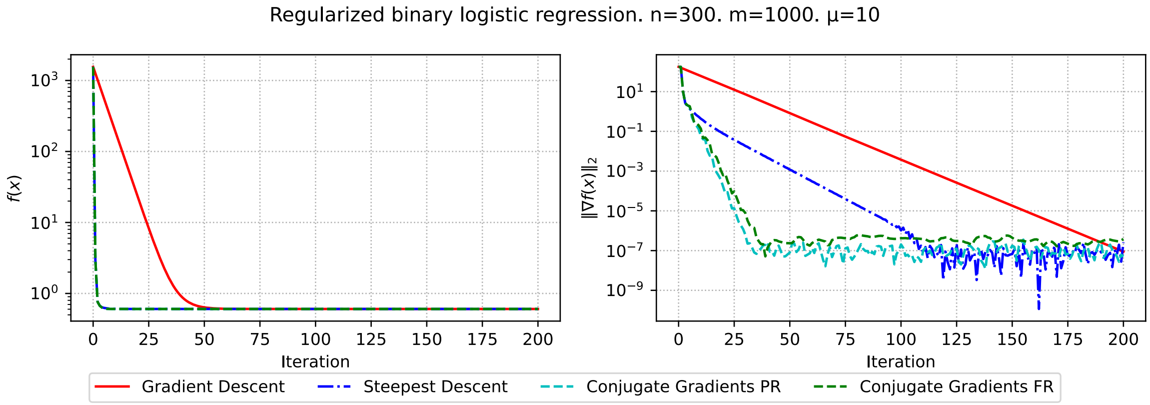

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Regularized binary logistic regression. n=300. m=1000. μ=10