

# Numerical Optimization

Lecture Notes #10  
Conjugate Gradient Methods — Linear CG, Part #1

Peter Blomgren,  
(blomgren.peter@gmail.com)

Department of Mathematics and Statistics  
Dynamical Systems Group  
Computational Sciences Research Center  
San Diego State University  
San Diego, CA 92182-7720

<http://terminus.sdsu.edu/>

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## Quick Recap: — Global Convergence and Enhancements

We looked at some theorems describing the convergence of our algorithms. We noted that there was a bit of a gap between what is generally true/practical, and what can be proved. (Theoretical limit points vs. numerical stopping criteria.)

Further, we looked at some enhancements including **scaling**

$$D = \text{diag}(d_1, d_2, \dots, d_n), \quad d_i > 0, \quad T(\Delta) = \{\bar{\mathbf{p}} \in \mathbb{R}^n : \|D\bar{\mathbf{p}}\| \leq \Delta\},$$

and the use of **non-Euclidean norms** — the latter primarily come in handy in the context of constrained optimization.

We now explore an important computational tool, which will help us solve problems of realistic size. — **Conjugate Gradient Methods.**



# Conjugate Gradient Methods: Introduction

For short: “**CG**” Methods.

- One of the most useful techniques for solving large linear systems of equations  $A\bar{x} = \bar{b}$ . “**Linear CG**”
- Can be adopted to solve nonlinear optimization problems. “**Nonlinear CG**” (Our type of problems!)
- Linear CG is an **alternative** to Gaussian elimination (well suited for large problems).
- Performance of linear CG is strongly tied to the distribution of the eigenvalues of  $A$ .

First, we explore the Linear CG method...

## The Linear CG Method

## Language and Notation

The **linear** CG method is an **iterative method** for solving linear systems of equations:

$$A\bar{\mathbf{x}} = \bar{\mathbf{b}}, \quad A \in \mathbb{R}^{n \times n}, \quad \bar{\mathbf{x}} \in \mathbb{R}^n, \quad \bar{\mathbf{b}} \in \mathbb{R}^n,$$

where the matrix  $A$  is **symmetric positive definite**<sup>∃ extensions</sup>.

Notice/Recall: This problem is **equivalent to minimizing**  $\Phi(\bar{\mathbf{x}})$  where

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

since

$$\nabla \Phi(\bar{\mathbf{x}}) = A\bar{\mathbf{x}} - \bar{\mathbf{b}} \stackrel{\text{def}}{=} \bar{\mathbf{r}}(\bar{\mathbf{x}}).$$

We refer to  $\bar{\mathbf{r}}(\bar{\mathbf{x}})$  as the **residual** of the linear system. Note that if  $\bar{\mathbf{x}}^* = A^{-1}\bar{\mathbf{b}}$ , then  $\bar{\mathbf{r}}(\bar{\mathbf{x}}^*) = 0$ , *i.e.* the residual is a measure of how close (or far) we are from solving the linear system.

## Conjugate Directions

### Definition (Conjugate Vector)

A set of nonzero vectors  $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \dots, \bar{\mathbf{p}}_{n-1}\}$  is said to be **conjugate** with respect to the symmetric positive definite matrix  $A$  if

$$\bar{\mathbf{p}}_i^T A \bar{\mathbf{p}}_j = 0, \quad \forall i \neq j.$$

### Property: Linear Independence of Conjugate Vectors

A set of conjugate vectors  $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \dots, \bar{\mathbf{p}}_{n-1}\}$  is **linearly independent**.



**Why should we care?** — We can minimize  $\Phi(\bar{\mathbf{x}})$  in  $n$  steps by successively minimizing along the directions in a conjugate set...

Conjugate Direction Method (  $\neq$  CG Method )

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Given a starting point  $\bar{\mathbf{x}}_0 \in \mathbb{R}^n$ , and a set of conjugate directions  $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \dots, \bar{\mathbf{p}}_{n-1}\}$  we generate a sequence of points  $\bar{\mathbf{x}}_k \in \mathbb{R}^n$  by setting

$$\bar{\mathbf{x}}_{k+1} = \bar{\mathbf{x}}_k + \alpha_k \bar{\mathbf{p}}_k,$$

where  $\alpha_k$  is the minimizer of the quadratic function  $\varphi(\alpha) = \Phi(\bar{\mathbf{x}}_k + \alpha \bar{\mathbf{p}}_k)$ , i.e. the minimizer of  $\Phi(\cdot)$  along the line  $\bar{\ell}(\alpha) = \bar{\mathbf{x}}_k + \alpha \bar{\mathbf{p}}_k$ .

We have already solved this problem — in the context of step-length selection for line search methods, **see** lecture #6 — so we “know” that the optimizer is given by

$$\alpha_k = -\frac{\bar{\mathbf{r}}_k^T \bar{\mathbf{p}}_k}{\bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_k}, \quad \text{where } \bar{\mathbf{r}}_k = \bar{\mathbf{r}}(\bar{\mathbf{x}}_k).$$

Conjugate Direction Method (  $\neq$  CG Method )

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Theorem ( $n$ -step convergence)

For any  $\bar{\mathbf{x}}_0 \in \mathbb{R}^n$  the sequence  $\{\bar{\mathbf{x}}_k\}$  generated by the conjugate direction algorithm converges to the solution  $\bar{\mathbf{x}}^*$  of the linear system in at most  $n$  steps.

The proof indicates how properties of CG are found...

## Proof: Part 1

(Fundamental Building Block).

Since the directions  $\{\bar{\mathbf{p}}_i\}$  are linearly independent, they must **span** the whole space  $\mathbb{R}^n$ . Hence, we can write

$$\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0 = \sum_{k=0}^{n-1} \sigma_k \bar{\mathbf{p}}_k$$

for some choice of scalars  $\sigma_k$ . We need to establish that  $\sigma_k = \alpha_k$ . □





Conjugate Direction Method (  $\neq$  CG Method )

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Proof: Part 2.

If we are generating  $\bar{\mathbf{x}}_k$  by the conjugate direction method, then we have

$$\bar{\mathbf{x}}_k = \bar{\mathbf{x}}_0 + \alpha_0 \bar{\mathbf{p}}_0 + \alpha_1 \bar{\mathbf{p}}_1 + \cdots + \alpha_{k-1} \bar{\mathbf{p}}_{k-1},$$

we multiply this by  $\bar{\mathbf{p}}_k^T A$ 

$$\bar{\mathbf{p}}_k^T A \bar{\mathbf{x}}_k = \bar{\mathbf{p}}_k^T A [\bar{\mathbf{x}}_0 + \alpha_0 \bar{\mathbf{p}}_0 + \alpha_1 \bar{\mathbf{p}}_1 + \cdots + \alpha_{k-1} \bar{\mathbf{p}}_{k-1}],$$

using the conjugacy property, we see that all but the first term on the right-hand-side are zero:

$$\bar{\mathbf{p}}_k^T A \bar{\mathbf{x}}_k = \bar{\mathbf{p}}_k^T A \bar{\mathbf{x}}_0 \quad \Leftrightarrow \quad \bar{\mathbf{p}}_k^T A (\bar{\mathbf{x}}_k - \bar{\mathbf{x}}_0) = 0.$$

Now we have

$$\bar{\mathbf{p}}_k^T A (\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0) = \bar{\mathbf{p}}_k^T A (\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0 - \underbrace{(\bar{\mathbf{x}}_k - \bar{\mathbf{x}}_0)}_{\text{adds 0}}) = \bar{\mathbf{p}}_k^T A (\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_k) = \bar{\mathbf{p}}_k^T (\bar{\mathbf{b}} - A \bar{\mathbf{x}}_k) = -\bar{\mathbf{p}}_k^T \bar{\mathbf{r}}_k.$$

□



Conjugate Direction Method (  $\neq$  CG Method )

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Proof: Part 3.

We have shown

$$\bar{\mathbf{p}}_k^T A(\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0) = -\bar{\mathbf{p}}_k^T \bar{\mathbf{r}}_k.$$

Now, we notice that the right-hand-side is the numerator in  $\alpha_k$ :

$$\alpha_k = \frac{-\bar{\mathbf{p}}_k^T \bar{\mathbf{r}}_k}{\bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_k} \Rightarrow \alpha_k = \frac{\bar{\mathbf{p}}_k^T A(\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0)}{\bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_k}.$$

We conclude the proof by showing that  $\sigma_k$  can be expressed in the same manner; we premultiply the expression for  $(\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0)$  by  $\bar{\mathbf{p}}_k^T A$  and obtain

$$\bar{\mathbf{p}}_k^T A(\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0) = \bar{\mathbf{p}}_k^T A \sum_{i=0}^{n-1} \sigma_i \bar{\mathbf{p}}_i = \sum_{i=0}^{n-1} \sigma_i \bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_i = \sigma_k \bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_k.$$

Hence,

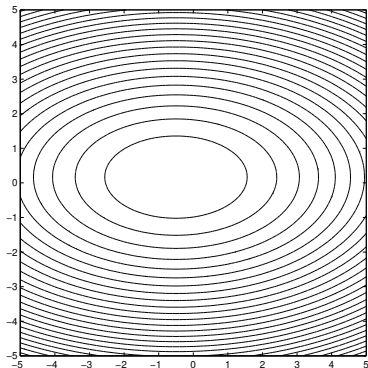
$$\sigma_k = \frac{\bar{\mathbf{p}}_k^T A(\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0)}{\bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_k} \equiv \alpha_k.$$



## Conjugate Direction Method: Comments and Interpretation

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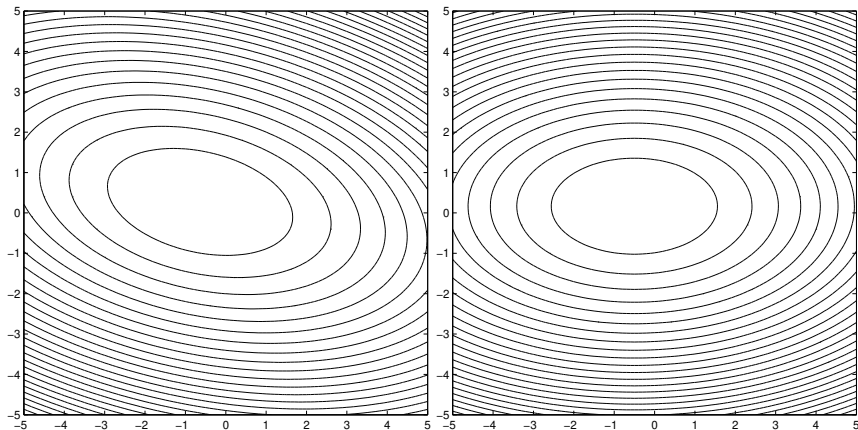
Most of the proofs regarding CD and CG methods are argued in a similar way — by looking at optimizers and residuals over sub-spaces of  $\mathbb{R}^n$  spanned by some subset of a set of conjugate vectors.



**Interpretation:** If the matrix  $A$  is diagonal, then the contours of  $\Phi(\bar{x})$  are ellipses whose axes are aligned with the coordinate directions. In this case, we can find the minimizer by performing 1D-minimizations along the coordinate directions  $\bar{e}_1, \bar{e}_2, \dots, \bar{e}_n$  in turn.

## Conjugate Direction Method: Comments and Interpretation

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**Interpretation (ctd.):** When  $A$  is not diagonal, the contours are still elliptical, but are no longer aligned with the coordinate axes. Successive minimization along the coordinate directions  $\bar{\mathbf{e}}_1, \bar{\mathbf{e}}_2, \dots, \bar{\mathbf{e}}_n$  can **not** guarantee convergence in  $n$  (or even a (fixed) finite number of) iterations.



Recovering  $n$ -step Convergence for Non-Diagonal  $A$ 

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For non-diagonal matrices  $A$ , the  $n$ -step convergence can be recovered by transforming the problem.

Let  $S \in \mathbb{R}^{n \times n}$  be a matrix with conjugate columns, i.e. if  $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \dots, \bar{\mathbf{p}}_{n-1}\}$  is a set of conjugate directions (with respect to  $A$ ), then

$$S = \begin{bmatrix} | & | & & | \\ \bar{\mathbf{p}}_0 & \bar{\mathbf{p}}_1 & \cdots & \bar{\mathbf{p}}_{n-1} \\ | & | & & | \end{bmatrix}.$$

We introduce a new variable  $\hat{\mathbf{x}} = S^{-1}\bar{\mathbf{x}}$ , and thus get the new quadratic objective which can be minimized in  $n$  steps

$$\hat{\Phi}(\hat{\mathbf{x}}) = \Phi(S\hat{\mathbf{x}}) = \frac{1}{2}\hat{\mathbf{x}}^T \underbrace{(S^T A S)}_{\text{Diagonal}} \hat{\mathbf{x}} - (S^T \bar{\mathbf{b}})^T \hat{\mathbf{x}}.$$

We note that the matrix  $(S^T AS)$  is diagonal by the conjugacy property, and that each coordinate direction  $\hat{\mathbf{e}}_i$  in  $\hat{\mathbf{x}}$ -space corresponds to the direction  $\bar{\mathbf{p}}_{i-1}$  in  $\bar{\mathbf{x}}$ -space.

When the matrix is diagonal, each coordinate minimization determines one of the components of the solution  $\bar{\mathbf{x}}^*$ . Hence, after  $k$  iterations, the quadratic has been minimized on the subspace spanned by  $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \dots, \hat{\mathbf{e}}_k$ .

If we instead minimize along the conjugate directions, then after  $k$  iterations, the quadratic has been minimized on the subspace spanned by  $\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \dots, \bar{\mathbf{p}}_{k-1}$ .

## Updating the Residual

Before we state a fundamental theorem regarding the conjugate direction method, we show the following lemma:

### Lemma

Given a starting point  $\bar{\mathbf{x}}_0 \in \mathbb{R}^n$  and a set of conjugate directions  $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \dots, \bar{\mathbf{p}}_{n-1}\}$  if we generate the sequence  $\bar{\mathbf{x}}_k \in \mathbb{R}^n$  by setting

$$\bar{\mathbf{x}}_{k+1} = \bar{\mathbf{x}}_k + \alpha_k \bar{\mathbf{p}}_k, \quad \text{where } \alpha_k = -\frac{\bar{\mathbf{r}}_k^T \bar{\mathbf{p}}_k}{\bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_k},$$

with  $\bar{\mathbf{r}}_k = A\bar{\mathbf{x}}_k - \mathbf{b}$ . Then the  $(k+1)$ st residual is given by the following expression

$$\bar{\mathbf{r}}_{k+1} = \bar{\mathbf{r}}_k + \alpha_k A \bar{\mathbf{p}}_k.$$

Proof:

(Quick One-Liner).

$$\bar{\mathbf{r}}_{k+1} = A\bar{\mathbf{x}}_{k+1} - \bar{\mathbf{b}} = A(\bar{\mathbf{x}}_k + \alpha_k \bar{\mathbf{p}}_k) - \bar{\mathbf{b}} = \alpha_k A \bar{\mathbf{p}}_k + (A\bar{\mathbf{x}}_k - \bar{\mathbf{b}}) = \alpha_k A \bar{\mathbf{p}}_k + \bar{\mathbf{r}}_k.$$



## Expanding Subspace Minimization

## Theorem (Expanding Subspace Minimization)

Let  $\bar{\mathbf{x}}_0 \in \mathbb{R}^n$  be any starting point and suppose that the sequence  $\{\bar{\mathbf{x}}_k\}$  is generated by

$$\bar{\mathbf{x}}_{k+1} = \bar{\mathbf{x}}_k + \alpha_k \bar{\mathbf{p}}_k, \quad \text{where } \alpha_k = -\frac{\bar{\mathbf{r}}_k^T \bar{\mathbf{p}}_k}{\bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_k}.$$

Then

$$\bar{\mathbf{r}}_k^T \bar{\mathbf{p}}_i = 0, \quad \text{for } i = 0, 1, \dots, k-1,$$

and  $\bar{\mathbf{x}}_k$  is the minimizer of  $\Phi(\bar{\mathbf{x}}) = \frac{1}{2} \bar{\mathbf{x}}^T A \bar{\mathbf{x}} - \bar{\mathbf{b}}^T \bar{\mathbf{x}}$  over the set

$$S(\bar{\mathbf{x}}_0, k) = \left\{ \bar{\mathbf{x}} : \bar{\mathbf{x}} = \bar{\mathbf{x}}_0 + \text{span}\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \dots, \bar{\mathbf{p}}_{k-1}\} \right\}.$$





## Expanding Subspace Minimization: Proof

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## Proof: Part 1

(Fundamental Building Block).

First, we show that a point  $\tilde{\mathbf{x}}$  minimizes  $\Phi$  over the set  $S(\bar{\mathbf{x}}_0, k)$  **if and only if**  $r(\tilde{\mathbf{x}})^T \bar{\mathbf{p}}_i = 0$ ,  $i = 0, 1, \dots, k-1$ .

Let  $h(\bar{\sigma}) = \Phi(\bar{\mathbf{x}}_0 + \sigma_0 \bar{\mathbf{p}}_0 + \sigma_1 \bar{\mathbf{p}}_1 + \dots + \sigma_{k-1} \bar{\mathbf{p}}_{k-1})$ . Since  $h(\bar{\sigma})$  is a strictly convex quadratic it has a unique minimizer  $\bar{\sigma}^*$  that satisfies

$$\frac{\partial h(\bar{\sigma}^*)}{\partial \sigma_i} = 0, \quad i = 0, 1, \dots, k-1$$

By the chain rule, this is equivalent to

$$\nabla \Phi(\underbrace{\bar{\mathbf{x}}_0 + \sigma_0^* \bar{\mathbf{p}}_0 + \sigma_1^* \bar{\mathbf{p}}_1 + \dots + \sigma_{k-1}^* \bar{\mathbf{p}}_{k-1}}_{\tilde{\mathbf{x}}})^T \bar{\mathbf{p}}_i = 0, \quad i = 0, 1, \dots, k-1$$

We recall that  $\nabla \Phi(\tilde{\mathbf{x}}) = A\tilde{\mathbf{x}} - \bar{\mathbf{b}} = \bar{\mathbf{r}}(\tilde{\mathbf{x}})$ , thus we have established  $\bar{\mathbf{r}}(\tilde{\mathbf{x}})^T \bar{\mathbf{p}}_i = 0 \Leftrightarrow \tilde{\mathbf{x}}$  minimizes  $\Phi$  over the set  $S(\bar{\mathbf{x}}_0, k)$ . □



## Expanding Subspace Minimization: Proof

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## Proof: Part 2.

We now show that the residuals  $\bar{\mathbf{r}}_k$  satisfy  $\bar{\mathbf{r}}_k^T \bar{\mathbf{p}}_i = 0$ ,  $i = 0, 1, \dots, k-1$ .

We use mathematical induction. Since  $\alpha_0$  is always the 1D-minimizer, we have  $\bar{\mathbf{r}}_1^T \bar{\mathbf{p}}_0 = 0$ , establishing the **base case**.

From the **inductive hypothesis**, that  $\bar{\mathbf{r}}_{k-1}^T \bar{\mathbf{p}}_i = 0$ ,  $i = 0, 1, \dots, k-2$ , we must show that  $\bar{\mathbf{r}}_k^T \bar{\mathbf{p}}_i = 0$ ,  $i = 0, 1, \dots, k-1$  in order to complete the proof.

From the lemma we have an expression for  $\bar{\mathbf{r}}_k = \bar{\mathbf{r}}_{k-1} + \alpha_{k-1} A \bar{\mathbf{p}}_{k-1}$ .

First off we have:  $\bar{\mathbf{p}}_{k-1}^T \bar{\mathbf{r}}_k = \bar{\mathbf{p}}_{k-1}^T \bar{\mathbf{r}}_{k-1} + \alpha_{k-1} \bar{\mathbf{p}}_{k-1}^T A \bar{\mathbf{p}}_{k-1} = 0$ , since, by construction (optimality)

$$\alpha_{k-1} = \frac{-\bar{\mathbf{p}}_{k-1}^T \bar{\mathbf{r}}_{k-1}}{\bar{\mathbf{p}}_{k-1}^T A \bar{\mathbf{p}}_{k-1}}$$



## Expanding Subspace Minimization: Proof

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## Proof: Part 3.

Finally,

$$\bar{\mathbf{p}}_i^T \bar{\mathbf{r}}_k = \bar{\mathbf{p}}_i^T \bar{\mathbf{r}}_{k-1} + \alpha_{k-1} \bar{\mathbf{p}}_i^T A \bar{\mathbf{p}}_{k-1} = 0, \quad i = 0, 1, \dots, k-2$$

since

$$\bar{\mathbf{p}}_i^T \bar{\mathbf{r}}_{k-1} = 0, \quad i = 0, 1, \dots, k-2$$

by the induction hypothesis, and

$$\bar{\mathbf{p}}_i^T A \bar{\mathbf{p}}_{k-1} = 0, \quad i = 0, 1, \dots, k-2$$

by conjugacy. This establishes  $\bar{\mathbf{p}}_i^T \bar{\mathbf{r}}_k = 0, i = 0, 1, \dots, k-1$ , which completes the proof. □

## Cliff-Hangers...

**Cliff-Hanger Questions:**

- How can we make this useful?
- Given  $A$ , how do we get a set of conjugate vectors? (They are not for sale at Costco!)
- Even if we have them, why is this scheme any better than Gaussian elimination?
- Where is the gradient?

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