# Numerical Optimization

## Lecture Notes #10

## Conjugate Gradient Methods — Linear CG, Part #1

Fall 2024

## Outline

1. Conjugate Gradient Methods
   - Introduction: Notation, Definitions, Properties
   - A Conjugate Direction Method
2. A Little Bit (More) Theory...
   - $n$-step Convergence for Non-Diagonal $A$; Cheap Residuals
   - Expanding Subspace Minimization

## Conjugate Gradient Methods: Introduction

For short: **"CG" Methods.**

- One of the most useful techniques for solving large linear systems of equations $A\bar{\mathbf{x}} = \bar{\mathbf{b}}$. **"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:

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

where the matrix $A$ is **symmetric positive definite**$^{\exists \text{ extensions}}$.

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

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

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 $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \ldots, \bar{\mathbf{p}}_{n-1}\}$ 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 $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \ldots, \bar{\mathbf{p}}_{n-1}\}$ 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 ( != CG Method )



Given a starting point $\bar{\mathbf{x}}_0 \in \mathbb{R}^n$, and a set of conjugate directions $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \ldots, \bar{\mathbf{p}}_{n-1}\}$ 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 ( != CG Method ) 

**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** (Fundmental Building Block).

## Conjugate Direction Method ( != CG Method )



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

**Proof: Part 1** (Fundmental 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 ( != CG Method ) 

**Proof: Part 2.**

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

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

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

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

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

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

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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 ( != CG Method ) 



### 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 $\alpha_k$:

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

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We conclude the proof by showing that $\sigma_k$ can be expressed in the same manner;

# Conjugate Direction Method ( != CG Method )



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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,

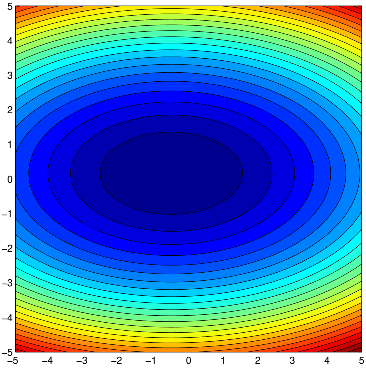
$$\sigma_k = \frac{\bar{\mathbf{p}}_k^T A(\bar{\mathbf{x}}^* - \bar{\mathbf{x}}_0)}{\bar{\mathbf{p}}_k^T A \bar{\mathbf{p}}_k} \quad \equiv \quad \alpha_k.$$

□

## Conjugate Direction Method: Comments and Interpretation



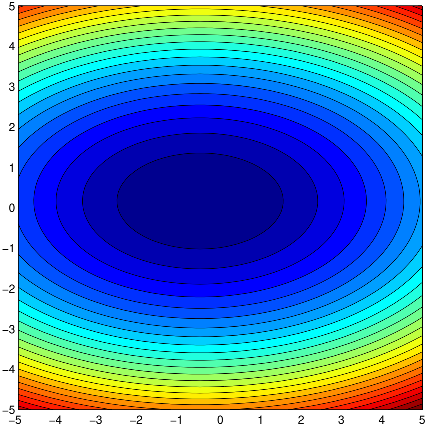
Most of the proofs regarding CD and CG methods are argued in a similar way — by looking at optimizers and residuals over sub-spaces of $\mathbb{R}^n$ spanned by some subset of a set of conjugate vectors.

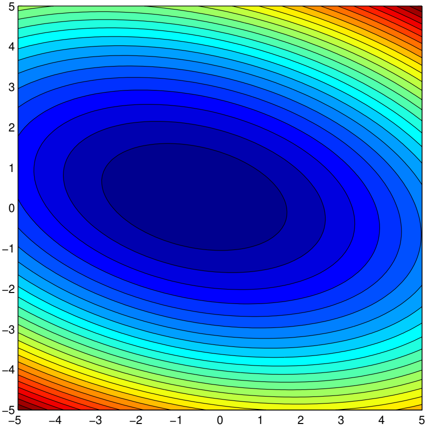



**Interpretation:** If the matrix $A$ is diagonal, then the contours of $\Phi(\bar{\mathbf{x}})$ are ellipses whose axes are aligned with the coordinate directions. In this case, we can find the minimizer by performing 1D-minimizations along the coordinate directions $\bar{\mathbf{e}}_1, \bar{\mathbf{e}}_2,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

# Conjugate Direction Method: Comments and Interpretation






**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 $\bar{\mathbf{e}}_1, \bar{\mathbf{e}}_2, \ldots, \bar{\mathbf{e}}_n$ can **not** guarantee convergence in $n$ (or even a (fixed) finite number of) iterations.

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



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 $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \ldots, \bar{\mathbf{p}}_{n-1}\}$ 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 $\widehat{\mathbf{x}} = S^{-1}\bar{\mathbf{x}}$, and thus get the new quadratic objective which can be minimized in $n$ steps

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

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



We note that the matrix $(S^T AS)$ is diagonal by the conjugacy property, and that each coordinate direction $\widehat{\mathbf{e}}_i$ in $\widehat{\mathbf{x}}$-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 $\widehat{\mathbf{e}}_1, \widehat{\mathbf{e}}_2, \ldots, \widehat{\mathbf{e}}_k$.

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

# 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 $\{\bar{\mathbf{p}}_0, \bar{\mathbf{p}}_1, \ldots, \bar{\mathbf{p}}_{n-1}\}$ if we generate the sequence $\bar{\mathbf{x}}_k \in \mathbb{R}^n$ by setting*

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

*with $\bar{\mathbf{r}}_k = A\bar{\mathbf{x}}_k - b$. 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).

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

### Proof: (Quick One-Liner).

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

$\square$

# 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*

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

*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*

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

# Expanding Subspace Minimization: Proof



## Proof: Part 1 (Fundmental 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 $r(\tilde{\mathbf{x}})^T \bar{\mathbf{p}}_i = 0$, $i = 0, 1, \ldots, k-1$.

## Expanding Subspace Minimization: Proof



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

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

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By the chain rule, this is equivalent to

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

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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



## Proof: Part 2.

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

# Expanding Subspace Minimization: Proof



## Proof: Part 2.

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

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

## Expanding Subspace Minimization: Proof



### Proof: Part 2.

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

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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



### Proof: Part 3.

Finally,

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

since

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

by the induction hypothesis, and

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

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

## 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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