

Reducing Memory Access Latencies using Data Compression in Sparse, Iterative Linear Solvers

An All-College Thesis

College of Saint Benedict/Saint John's University

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April 2018

Project Title: Reducing Memory Access Latencies using Data
Compression in Sparse, Iterative Linear Solvers
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Abstract

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1 Introduction

2 Background

2.1 Conjugate Gradient

Conjugate Gradient is the iterative solver used by HPCG [1]. Symmetric, positive definite matrices will guarantee the converge of Conjugate Gradient to the correct solution within n iterations, where n is the number of dimensions, when using exact algebra [4]. More importantly, Conjugate Gradient can be used as in iterative method, providing a solution, \vec{x} , where $\|\mathbf{A}\vec{x} - \vec{b}\|$ is within some tolerance, after significantly fewer than n iterations, allowing it to find solutions to problems where even n iterations is infeasible [5].

To understand the Conjugate Gradient, first consider the quadratic form of $\mathbf{A}\vec{x} = \vec{b}$. The quadratic form is a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ where

$$f(\vec{x}) = \frac{1}{2}\vec{x}^T \mathbf{A} \vec{x} - \vec{b} \cdot \vec{x} + c \quad (1)$$

for some $c \in \mathbb{R}$. Note that

$$\nabla f(\vec{x}) = \frac{1}{2}(\mathbf{A} + \mathbf{A}^T)\vec{x} - \vec{b}$$

Then, when \mathbf{A} is symmetric,

$$\nabla f(\vec{x}) = \mathbf{A}\vec{x} - \vec{b}$$

So, the solution to $\mathbf{A}\vec{x} = \vec{b}$ is the sole critical point of f [3]. Since \mathbf{A} is the Hessian matrix of f at the point, if \mathbf{A} is positive definite, then that critical point is a minimum. Thus, if \mathbf{A} is a symmetric, positive definite matrix, then the minimum of f is the solution to $\mathbf{A}\vec{x} = \vec{b}$ [5].

The method of Steepest Decent is useful for understanding Conjugate Gradient, because they both use a similar approach to minimize Equation 1, and thus solve $\mathbf{A}\vec{x} = \vec{b}$. This shared approach is to take an initial \vec{x}_0 and move downwards in the steepest direction, within certain constraints, of the surface defined by Equation 1 [3]. Because the gradient at a point is the direction of maximal increase, \vec{x} should be moved in the opposite direction of the gradient. Thus, to compute the next value of \vec{x} , use

$$\vec{x}_{i+1} = \vec{x}_i + \alpha_i \vec{r}_i \quad (2)$$

for some $\alpha_i > 0$ and where $\vec{r}_i = -\nabla f(\vec{x}_i) = \vec{b} - \mathbf{A}\vec{x}_i$ is the residual of \vec{x}_i . Since $\mathbf{A}\vec{x} = \vec{b}$ is the only critical point and a minimum of the quadratic function, f , the ideal value of α_i is the one that minimizes $f(\vec{x}_{i+1})$. Thus, choose α_i such that

$$\begin{aligned} 0 &= \frac{d}{d\alpha_i} f(\vec{x}_{i+1}) \\ &= \frac{d}{d\alpha_i} f(\vec{x}_i + \alpha \vec{r}_i) \\ \alpha_i &= \frac{\vec{r}_i \cdot \vec{r}_i}{\vec{r}_i \cdot \mathbf{A} \vec{r}_i} \end{aligned}$$

Note that by using Equation 2, we can derive

$$\vec{r}_{i+1} = \vec{r}_i - \alpha \mathbf{A} \vec{r}_i. \quad (3)$$

Because $\mathbf{A} \vec{r}_i$ is already computed to find α_i , using Equation 3 to compute the residual results in one less matrix-vector product per iteration. The steps for the Method of Steepest Decent are

$$\begin{aligned} \vec{r}_0 &= \vec{b} - \mathbf{A} \vec{x}_0 \\ \alpha_i &= \frac{\vec{r}_i \cdot \vec{r}_i}{\vec{r}_i \cdot \mathbf{A} \vec{r}_i} \\ \vec{x}_{i+1} &= \vec{x}_i + \alpha_i \vec{r}_i \\ \vec{r}_{i+1} &= \vec{r}_i - \alpha \mathbf{A} \vec{r}_i \end{aligned}$$

until $\|\vec{r}_i\|$ is less than some tolerance [5].

Example 1. Consider the linear system

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix}, \quad \vec{b} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}$$

and use $c = 0$. Note that the solution is

$$\vec{x} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}.$$

When starting at the origin, the iteration of Method of Steepest Decent becomes

$\vec{x}_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$	$\vec{r}_0 = \begin{bmatrix} 5 \\ 5 \end{bmatrix}$	$\alpha_0 = 2/7$
$\vec{x}_1 = \begin{bmatrix} 10/7 \\ 10/7 \end{bmatrix}$	$\vec{r}_1 = \begin{bmatrix} 5/7 \\ -5/7 \end{bmatrix}$	$\alpha_1 = 2/3$
$\vec{x}_2 = \begin{bmatrix} 40/21 \\ 20/21 \end{bmatrix}$	$\vec{r}_2 = \begin{bmatrix} 5/21 \\ 5/21 \end{bmatrix}$	$\alpha_2 = 2/7$
$\vec{x}_3 = \begin{bmatrix} 290/147 \\ 50/49 \end{bmatrix}$	$\vec{r}_3 = \begin{bmatrix} 5/147 \\ -5/147 \end{bmatrix}$	$\alpha_3 = 2/3$
\vdots	\vdots	\vdots

The \vec{x}_i 's are plotted with a contour graph of the quadratic form in Figure 1.

The Conjugate Directions family of linear solvers, of which Conjugate Gradient is a member of, attempts to improve on the number of iterations needed by Steepest Decent. [5]. Note that, in Example 1, the directions of \vec{r}_0 and \vec{r}_2 are the same and the directions of \vec{r}_1 and \vec{r}_3 are the same. Thus, the same direction has to be traversed multiple times. Additionally, note that the two sets of residual directions are perpendicular to each other. Conjugate Directions attempts

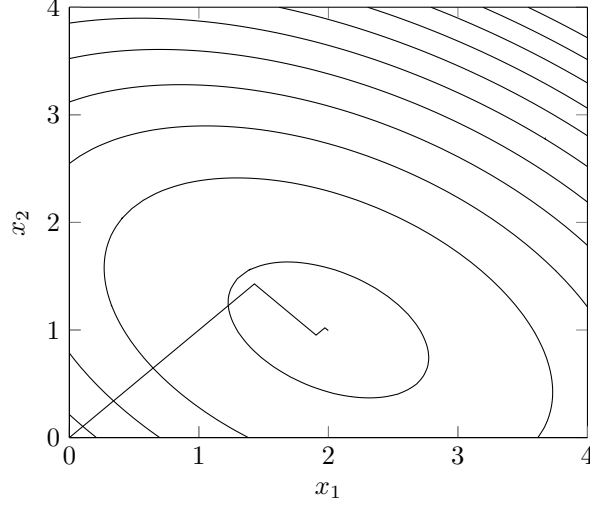


Figure 1: Contour graph of the quadratic function and the first six values of \vec{x} produced by steepest descent for Example 1

to improve on this, by making the search directions, $\vec{d}_0, \vec{d}_1, \dots$, \mathbf{A} -orthogonal to each other and only moving \vec{x} once in each search direction. Two vectors, \vec{u}, \vec{v} are \mathbf{A} -orthogonal, or conjugate, if $\vec{u}^T \mathbf{A} \vec{v} = 0$. The requirement for Conjugate Directions is to make \vec{e}_{i+1} \mathbf{A} -orthogonal to \vec{d}_i , where $\vec{e}_i = \vec{x}_i - \mathbf{A}^{-1} \vec{b}$ is the error of \vec{x}_i . The computation of α_i changes to find the minimal value along \vec{d}_i instead of \vec{r}_i .

$$\alpha_i = \frac{\vec{d}_i^T \vec{r}_i}{\vec{d}_i^T \mathbf{A} \vec{d}_i}.$$

Conjugate Gradient is a form of Conjugate Directions where the residuals are made to be \mathbf{A} -orthogonal to each other. This is done using the Conjugate Gram-Schmidt Process. To do this, each search direction, \vec{d}_i is computed by taking \vec{r}_i and removing any components that are not \mathbf{A} -orthogonal to the previous \vec{d} 's. So, let $\vec{d}_0 = \vec{r}_0$ and for $i > 0$ let

$$\vec{d}_i = \vec{r}_i + \sum_{k=0}^{i-1} \beta_{(i,k)} \vec{d}_k$$

with $\beta_{(i,k)}$ defined for $i > k$. Then, solving for $\beta_{(i,k)}$ gives

$$\beta_{(i,k)} = -\frac{\vec{r}_i \cdot \mathbf{A} \vec{d}_k}{\vec{d}_k \cdot \mathbf{A} \vec{d}_k}.$$

Note that each residual is orthogonal to the previous search directions, and thus the previous residuals. So, it can be shown that \vec{r}_{i+1} is \mathbf{A} -orthogonal to

all previous search directions, except \vec{d}_i [5]. Then, $\beta_{(i,k)} = 0$ for $i - 1 \neq k$. To simplify notation, let $\beta_i = \beta_{(i,i-1)}$. So, each new search direction can then be computed by

$$\vec{d}_i = \vec{r}_i + \beta_i \vec{d}_{i-1}.$$

This results in the following steps for Conjugate Gradient

$$\begin{aligned} \vec{d}_0 &= \vec{r}_0 = \vec{b} - \mathbf{A}\vec{x}_0 \\ \alpha_i &= \frac{\vec{r}_i \cdot \vec{r}_i}{\vec{d}_i \cdot \mathbf{A}\vec{d}_i} \\ \vec{x}_{i+1} &= \vec{x}_i + \alpha_i \vec{d}_i \\ \vec{r}_{i+1} &= \vec{r}_i - \alpha_i \mathbf{A}\vec{d}_i \\ \beta_{i+1} &= \frac{\vec{r}_{i+1} \cdot \vec{r}_{i+1}}{\vec{r}_i \cdot \vec{r}_i} \\ \vec{d}_{i+1} &= \vec{r}_{i+1} + \beta_{i+1} \vec{d}_i \end{aligned}$$

continuing the iteration until $\|\vec{r}_i\|$ is less than the specified tolerance.

Example 2. Consider the linear system used in Example 1 where

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix}, \quad \vec{b} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}.$$

The result of applying Conjugate Gradient is

$$\begin{aligned} \vec{x}_0 &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} & \vec{r}_0 &= \begin{bmatrix} 5 \\ 5 \end{bmatrix} & \vec{d}_0 &= \begin{bmatrix} 5 \\ 5 \end{bmatrix} & \alpha_0 &= 2/7 \\ \vec{x}_1 &= \begin{bmatrix} 10/7 \\ 10/7 \end{bmatrix} & \vec{r}_1 &= \begin{bmatrix} 5/7 \\ -5/7 \end{bmatrix} & \beta_1 &= 1/49 & \vec{d}_1 &= \begin{bmatrix} 40/49 \\ -30/49 \end{bmatrix} & \alpha_1 &= 7/10 \\ \vec{x}_2 &= \begin{bmatrix} 2 \\ 1 \end{bmatrix} & \vec{r}_2 &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} \end{aligned}$$

Note that after two iterations, \vec{x} reaches the exact solution, compared to the iterations of Steepest Decent in Example 1. Figure 2 shows the values of \vec{x} with the contour graph of the quadratic function.

2.2 Multigrid Preconditioner with Gauss-Seidel Step

2.3 Problem Setup of High Performance Conjugate Gradient

The problem used to create the linear system used by HPCG, and thus by this project, is a three dimensional partial differential equation (PDE) model [1]. This problem is approximating the function $u(x, y, z)$ over the three dimensional rectangular region $\Omega \in \mathbb{R}^3$ such that

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0,$$

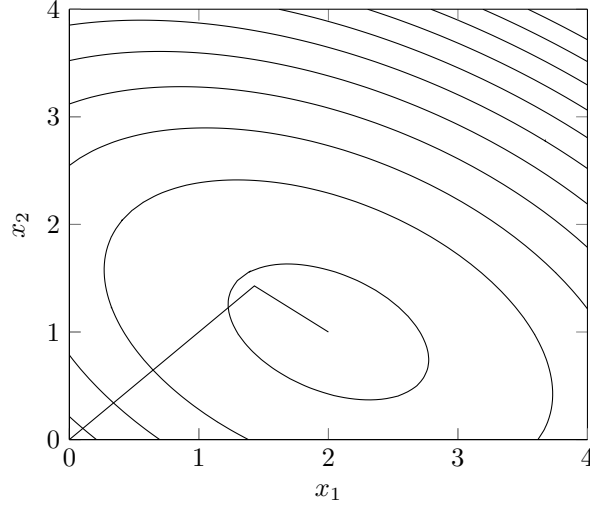


Figure 2: Contour graph of the quadratic function and the each value of \vec{x} produced by Conjugate Gradient for Example 2

with $u(x, y, z) = 1$ along the boundaries of Ω . Note that the solution is $u(x, y, z) = 1$ over Ω . The linear system is created by using the finite difference method with a 27-point stencil on the PDE over a rectangular grid with nodes of fixed distance. The matrix's diagonal consists of the value 26, and -1's fill the entries for the row's 26 grid neighbors. The right hand side of the equation has a value of 14 for corner points, 12 for edge points, 9 for side points and 0 for interior points [2]. The solution vector consists of all 1's.

HPCG uses an implementation of Conjugate Gradient algorithm with a multigrid preconditioner variant [1]. As HPCG is designed to emulate the performance characteristics of real world problems with out needing to be a robust solver, it only uses 3 levels of grid coarseness with only a single smoother pass at the coarsest grid level. The multigrid uses a symmetric Gauss-Seidel step as the smoother. The restriction operation simply samples half the points in dimension, resulting in a reduction of grid size by a factor of eight in each level of coarseness. To prolong the coarse grids, each coarse point is added to the fine point in was sampled from. The zero vector is used as the overall initial guess for x , as well as the initial guess for each grid level in the multigrid cycle.

2.4 Data Access Patterns of High Performance Conjugate Gradient

2.5 Compression Strategies

Numerous compression strategies were considered for this project. Figure 3 lists the compressions tried for each main data structure. Note that most compress-

Strategy	Vector Values	Matrix Values	Matrix Indices
Single Precision	Yes	Yes	Not Able
Mixed Precision	Yes	Not Able	Not Able
1 Bit	Not Able	Yes	Not Able
Squeeze (SZ)	Yes	Yes	Yes
ZFP	Yes	Yes	No
Elias Gamma	Not Able	Not Able	Yes
Elias Delta	Not Able	Not Able	Yes
Huffman	Not Able	No	Yes
Op Code	Not Able	Not Able	Yes

Figure 3: Overview of Compression Strategies

sion methods were only used with one or two of the data types, even if able to be reasonably used within the constraints of additional data.

2.5.1 Restrictions on Compression Strategies

2.5.2 Single and Mixed Precision Floating Point Numbers

2.5.3 1 bit Compression

2.5.4 Squeeze (SZ) Compression

2.5.5 ZFP Compression

2.5.6 Elias Gamma Coding and Delta Coding

2.5.7 Op-Code Compression

2.5.8 Huffman Coding

2.5.9 Combined Compression Strategies

3 Test Results

4 Conclusions and Future Work

5 References

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