Iterative Solvers for Linear Systems using a Minimization Approach

Martin Berzins
School of Computing

Aim to introduce better methods for solving sub-classes of Ax=b

Consider Gradient Descent - very widely used in deep learning

Introduce Conjugate Gradient methods



Symmetric Positive Definite Matrices

Symmetric matrices entries $A_{ij} = A_{ji}$

Positive definite matrices $x^T A x \ge 0$ for all x

Minimize $\frac{1}{2}x^T Ax - x^T b$ instead of solving Ax - b = 0

at a minimum Ax - b

Differentiate $\frac{1}{2} x^T A x - x^T b$ wrt components

of x and set to zero giving Ax - b.



Quadratic Form Example

$$\begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ -8 \end{bmatrix}$$

Quadratic form

$$Q(x_1, x_2) = \frac{1}{2} \begin{bmatrix} x_1, x_2 \end{bmatrix} \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} 2x_1 - 8x_2 \end{bmatrix} = 0$$

Expanding

$$Q(x_1, x_2) = \frac{1}{2} [3x_1^2 + 4x_1x_2 + 6x_2^2] - [2x_1 - 8x_2] = 0$$

Differentiate $Q(x_1, x_2)$ wrt x_1 and $Q(x_1, x_2)$ wrt x_2 and set to zero to get original eqns at minimum

$$\frac{1}{2}[6x_1 + 4x_2] - 2 = 0 \qquad \frac{1}{2}[4x_1 + 12x_2] + 8 = 0$$



Gradient Vector

Suppose that we have a function that depends on two or more variables

$$Q(x_1, x_2) = \frac{1}{2} [3x_1^2 + 4x_1x_2 + 6x_2^2] - [2x_1 - 8x_2] = 0$$

Then the gradient vector is defined by

$$\nabla Q = \begin{bmatrix} \frac{\partial Q}{\partial x_1} \\ \frac{\partial Q}{\partial x_2} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} [6x_1 + 4x_2] - 2 \\ \frac{1}{2} [4x_1 + 12x_2] + 8 \end{bmatrix} = Ax - b$$

The operation $\frac{\partial Q}{\partial x_1}$ means differentiate Q with respect to x_1

The operation $\frac{\partial Q}{\partial x_2}$ means differentiate Q with respect to x_2



Stationary and non Stationary Iterative Methods

The problem is still to solve for Ax = b

Stationary (or relaxation) methods:

$$\mathbf{x}^{(i+1)} = \mathbf{G}\mathbf{x}^{(i)} + \mathbf{c}$$

where **G** and **c** do not depend on iteration count i

Non-stationary methods:

$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} + \alpha^{(i)} \mathbf{p}^{(i)}$$

where computation involves information that changes at each iteration



Main Idea – Search Directions

Construct Search Directions based on residuals to be orthogonal.

$$(r^{(i)})^T . r^{(i+1)} = 0$$

- This means that the residual vectors may span the vector space that the solution is in
- E.g. in three dimensions the solution may be expressed as

$$x_{solution} = x^{(0)} + \alpha_1 r^{(1)} + \alpha_2 r^{(2)} + \alpha_3 r^{(3)}$$

- We then search along these directions
- For the steepest descent method the $\chi^{(0)}$ search directions are only locally orthogonal.



Steepest Descent Algorithm

Iteratively update x along the gradient direction

$$r(x) = \mathbf{b} - \mathbf{A}\mathbf{x}$$

The stepsize is selected to minimize $f(\mathbf{x})$ along $-r(\mathbf{x})$

Set i=0,
$$\epsilon > 0$$
, $\mathbf{x}^{(0)} = \mathbf{0}$, so $\mathbf{r}^{(0)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(0)} = \mathbf{b}$

While $||\mathbf{r}^{(i)}|| \ge \varepsilon$ Do

(a) calculate the best stepsize $\alpha^{(i)} = \frac{\left[r^{(i)}\right]^T r^{(i)}}{\left[r^{(i)}\right]^T A r^{(i)}}$

(b)
$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} + \alpha^{(i)} \mathbf{r}^{(i)}$$

(c)
$$\mathbf{r}^{(i+1)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(i+1)}$$

$$(d) i := i + 1$$

End While



Eliminating a matrix multiplication

Matrix vector multiplications are the main work of an iterative algorithm,

$$r^{i+1} = b - Ax^{i+1}$$

$$as$$

$$x^{i+1} = x^{i} + \alpha^{(i)}r^{(i)}$$

$$r^{i+1} = b - A(x^{i} + \alpha^{(i)}r^{(i)})$$

$$r^{i+1} = r^{(i)} - \alpha^{(i)}Ar^{(i)}$$

As we need $Ar^{(i)}$ elsewhere we only need one matrix multiplication per step.



Choosing step α

The current gradient is $b - Ax^{i+1}$

$$r^{(i+1)} = r^{(i)} - \alpha^{(i)} A r^{(i)}$$

As we require that the gradients are orthogonal at each step

$$(r^{(i)})^T r^{(i+1)} = 0$$

and so we require

$$(r^{(i)})^T r^{(i+1)} = (r^{(i)})^T r^{(i)} - \alpha^{(i)} (r^i)^T A r^{(i)} = 0$$

or that

$$(r^{(i)})^T r^{(i)} = \alpha^{(i)} (r^i)^T A r^{(i)} \Rightarrow \alpha^{(i)} = \frac{(r^{(i)})^T r^{(i)}}{(r^i)^T A r^{(i)}}$$



Steepest Descent Algorithm

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Set i=0,
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While $||\mathbf{r}^{(i)}|| \ge \varepsilon$ Do

(a) calculate the best stepsize $\alpha^{(i)} = \frac{\left[r^{(i)}\right]^T r^{(i)}}{\left[r^{(i)}\right]^T A r^{(i)}}$

(b)
$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} + \alpha^{(i)} \mathbf{r}^{(i)}$$

(c)
$$\mathbf{r}^{(i+1)} = \mathbf{r}^{(i)} - \alpha^{(i)} \mathbf{A} \mathbf{r}^{(i)}$$

(d)
$$i := i + 1$$

End While

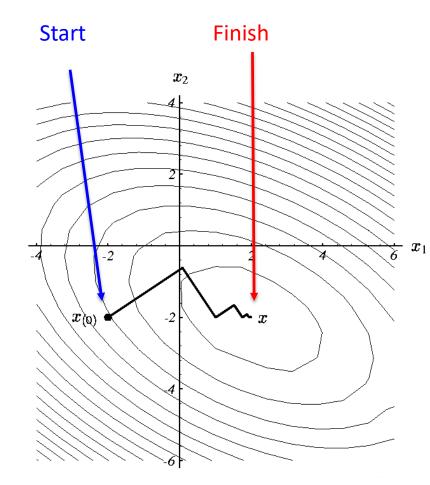
Note there is only one matrix, vector multiply per iteration



SD Example

$$\begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ -8 \end{bmatrix}$$

iter	\mathbf{X}_1	\mathbf{X}_2	\mathbf{r}_{1}	r_2	α
0	0.000	0.000	2.000	-8.000	0.243
1	0.410	-1.639	4.048	1.012	0.205
2	1.393	-1.393	0.607	-2.429	0.243
3	1.517	-1.890	1.229	0.307	0.205
4	1.816	-1.816	0.184	-0.737	0.243
5	1.853	-1.967	0.373	0.093	0.205
6	1.944	-1.944	0.056	-0.224	0.243
7	1.955	-1.990	0.113	0.028	0.205
8	1.983	-1.983	0.017	-0.068	0.243



Steepest Descent Code

```
%% Steepest Descent example
A = [3 \ 2; 2 \ 6]
b = [2 -8]
x = [0 \ 0]'
r = b;
normVal=Inf;
itr = 0;
tol = 0.1e-1;
%% Algorithm%%
while normVal>tol
    xold=x;
    y = A*r;
    alpha = (r'*r)/(r'*y);
    x = x + alpha*r;
    r = r - alpha* y;
    itr=itr+1;
    normVal=abs(xold-x);
end
```



Additional Material on Machine Learning Applications of Gradient Descent

The following material is to give you an overview of some aspects of gradient descent use in machine learning. The material is not related to any of the assignments



Improvements in Gradient Descent

- Back-tracking is used to make sure that the function decreases at each step
- The gradient may be evaluated at different points this is Nesterov's method
- The Lasso Method may be used to make sure the solution is in a valid solution space
- This is a very fast moving and active research area right now
- These ideas are all discussed in Linear Algebra and Learning from Data Gilbert Strang MIT Press 2019

Widely used in deep learning

Only randomly makes use of parts of the residual

Very slow but reliable Eventually get to a solution

Original method – Robbins and Munro Annals of Math. Stats vol.22 1951 pp400-407

Modern GPU architectures make large amounts of computation routine



Machine learning: usually minimizing the in-sample loss (training loss)

$$\min_{\boldsymbol{w}} \{ \frac{1}{N} \sum_{n=1}^{N} \ell(\boldsymbol{w}^T \boldsymbol{x}_n, y_n) \} := E_{\text{in}}(\boldsymbol{w}) \text{ (linear model)}$$

$$\min_{\boldsymbol{w}} \{ \frac{1}{N} \sum_{n=1}^{N} \ell(h_{\boldsymbol{w}}(\boldsymbol{x}_n), y_n) \} := E_{\text{in}}(\boldsymbol{w}) \text{ (general hypothesis)}$$

 ℓ : loss function (e.g., $\ell(a,b)=(a-b)^2$)

Gradient descent:

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \underbrace{\nabla E_{\mathsf{in}}(\mathbf{w})}_{\mathsf{Main computation}}$$

• In general, $E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} f_n(\mathbf{w})$, each $f_n(\mathbf{w})$ only depends on (\mathbf{x}_n, y_n)



Gradient:

$$\nabla E_{\rm in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \nabla f_n(\mathbf{w})$$

- Each gradient computation needs to go through all training samples slow when millions of samples
- Faster way to compute "approximate gradient"?



Gradient:

$$\nabla E_{\rm in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \nabla f_n(\mathbf{w})$$

- Each gradient computation needs to go through all training samples slow when millions of samples
- Faster way to compute "approximate gradient"?
- Use stochastic sampling:
 - Sample a small subset $B \subseteq \{1, \dots, N\}$
 - Estimate gradient

$$\nabla E_{\mathsf{in}}(\boldsymbol{w}) \approx \frac{1}{|B|} \sum_{n \in B} \nabla f_n(\boldsymbol{w})$$

|B|: batch size



- Input: training data $\{x_n, y_n\}_{n=1}^N$
- Initialize w (zero or random)
- For $t = 1, 2, \cdots$
 - Sample a small batch $B \subseteq \{1, \dots, N\}$
 - Update parameter

$$\mathbf{w} \leftarrow \mathbf{w} - \eta^t \frac{1}{|B|} \sum_{n \in B} \nabla f_n(\mathbf{w})$$



- In gradient descent, η (step size) is a fixed constant
- Can we use fixed step size for SGD?
- SGD with fixed step size cannot converge to global/local minimizers
- If \mathbf{w}^* is the minimizer, $\nabla f(\mathbf{w}^*) = \frac{1}{N} \sum_{n=1}^{N} \nabla f_n(\mathbf{w}^*) = 0$,

but
$$\frac{1}{|B|} \sum_{n \in B} \nabla f_n(\mathbf{w}^*) \neq 0$$
 if B is a subset

(Even if we got minimizer, SGD will move away from it)

To make SGD converge:

Step size should decrease to 0

$$\eta^t o 0$$

Usually with polynomial rate: $\eta^t pprox t^{-a}$ with constant a

Stochastic Gradient Descent as Used Today

- Gradients are computed using back propagation a previously computed gradient is used. – ADAGRAD and ADAM methods
- Instead of least squares objective function hinge loss or cross entropy loss are used
- Randomized Kaczmarz method is a very efficient update method.
- Averaging values over multiple iterations holds promise, - Stocastiv Weight Averaging SWA.
- Again this is a very fast moving and active research area right now
- These ideas are all discussed in Linear Algebra and Learning from Data Gilbert Strang MIT Press 2019



Gradient Descent vs Stochastic Gradient Descent

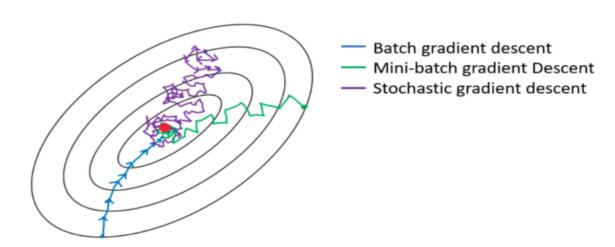
Stochastic gradient descent:

pros:

cheaper computation per iteration faster convergence in the beginning

cons:

less stable, slower final convergence hard to tune step size



(Figure from https://medium.com/@ImadPhd/gradient-descent-algorithm-and-its-variants-10f652806a3)



Main Material restarts here



Conjugate Direction Methods

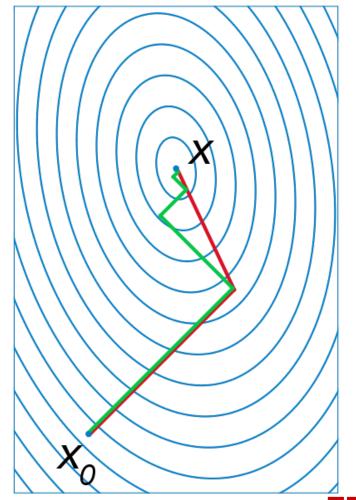
An improvement over the steepest descent is to take the exact number

of steps using a set of search directions and obtain the solution after *n* such steps

This is the basic idea in the conjugate direction methods

Image compares steepest
descent with a conjugate
direction approach

An example of a conjugate directions type Method is the Conjugate Gradient method

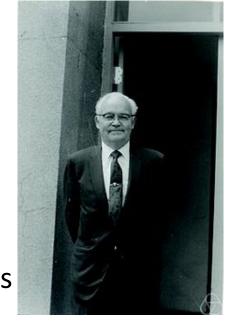




Conjugate Gradient Method

A is positive definite if for every nonzero vector v and its transpose v^T , the product $v^T Ax > 0$

If A is symmetric and positive definite, then the function



Magnus Hestenes

$$q(v) = \frac{1}{2}v^T A v - v^T b + c$$

has a unique minimizer that is solution to Av = bConjugate gradient is an iterative method that solves Av = bby minimizing q(x).

Minimization involves picking orthogonal search directions $d_{\scriptscriptstyle k}$

Pick
$$v_1$$

Conjugate Gradient Algorithm

Let
$$r_1 = b - Av_1$$
 first residual $d_1 = r_1$ pick first direction

For
$$k = 1, 2, 3, n$$

$$q_k = Ad_k$$

$$\alpha_k = \frac{r_k . r_k}{d_k . q_k}$$
 pick distance along search direction

$$v_{k+1} = v_k + \alpha_k d_k$$
 new value

$$\mathbf{r}_{k+1} = r_k - \alpha_k q_k$$
 new residual

$$\beta_k = \frac{r_{k+1}.r_{k+1}}{r_k.r_k}$$

$$d_{k+1} = r_{k+1} + \beta_k d_k$$
 new search direction

end

```
function x=cgm(A,b,sol)
% set CGM parameters
tol=1000*eps;
nm=length(b);
x=zeros(nm,1);
Tic
% start iteration
r=b-A*x; d=r;
rr=dot(r,r);
counter=0; err=1;
```

"Simple" Example Code

```
while err>tol
  counter=counter+1;
  iter(counter)=counter;
  if counter==1
    beta=0;
  else
    beta=rr/rr0;
  end;
  d=r+beta*d;
  q=A*d;
  alpha=rr/dot(d,q);
  x=x+alpha*d;
  r0=r;
  r=r-alpha*q;
  rr0=rr;
  rr=dot(r,r);
  error2(counter)=norm(alpha*d,inf);
  error3(counter)=norm(r,inf);
  error(counter)=norm(x-sol,inf);
  err=error(counter);
end;
toc
```

Using the same system as before, let

$$\mathbf{A} = \begin{bmatrix} 10 & -5 & -4 \\ -5 & 12 & -6 \\ -4 & -6 & 10 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 10 \\ -20 \\ 15 \end{bmatrix}$$
 We are solving for $\mathbf{x} = \begin{bmatrix} 3.354 \\ 1.645 \\ 3.829 \end{bmatrix}$

- Select i=0, $\mathbf{x}^{(0)} = \mathbf{0}$, $\epsilon = 0.1$, then $\mathbf{r}^{(0)} = \mathbf{b}$
- With i = 0, $d^{(0)} = r^{(0)} = b$

$$\alpha^{(0)} = \frac{(d^{(0)})' r^{(0)}}{(d^{(0)})' A d^{(0)}} = 0.0582$$

$$\mathbf{x}^{(I)} = \mathbf{x}^{(0)} + \alpha^{(0)} \mathbf{d}^{(I)} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} + 0.0582 \times \begin{bmatrix} 10 \\ -20 \\ 15 \end{bmatrix} = \begin{bmatrix} 0.582 \\ -1.165 \\ 0.873 \end{bmatrix}$$

$$\mathbf{r}^{(I)} = \mathbf{r}^{(0)} - \alpha^{(0)} \mathbf{A} \mathbf{d}^{(I)} = \begin{bmatrix} 10 \\ -20 \\ 15 \end{bmatrix} - 0.0582 \times \begin{bmatrix} 10 & -5 & -4 \\ -5 & 12 & -6 \\ -4 & -6 & 10 \end{bmatrix} \begin{bmatrix} 10 \\ -20 \\ 15 \end{bmatrix} = \begin{bmatrix} 1.847 \\ 2.129 \\ 1.606 \end{bmatrix}$$

$$i = i + 1 = 1$$

This first step exactly matches Steepest Descent

With i=1 solve for $\beta^{(1)}$

$$\beta^{(2)} = \frac{\left[\mathbf{r}^{(1)}\right]^T \mathbf{r}^{(1)}}{\left[\mathbf{r}^{(0)}\right]^T \mathbf{r}^{(0)}} = \frac{10.524}{725} = 0.01452$$

$$\mathbf{d}^{(2)} = \mathbf{r}^{(1)} + \boldsymbol{\beta}^{(2)} \mathbf{d}^{(1)} = \begin{bmatrix} 1.847 \\ 2.128 \\ 1.606 \end{bmatrix} + 0.01452 \times \begin{bmatrix} 10 \\ -20 \\ 15 \end{bmatrix} = \begin{bmatrix} 1.992 \\ 1.838 \\ 1.824 \end{bmatrix}$$

Then

$$\alpha^{(1)} = \frac{(d^{(1)})' r^{(1)}}{(d^{(1)})' A d^{(1)}} = \frac{725}{12450} = 1.388$$

And

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \alpha^{(1)}\mathbf{d}^{(2)} = \begin{bmatrix} 0.582 \\ -1.165 \\ 0.873 \end{bmatrix} + 1.388 \times \begin{bmatrix} 1.993 \\ 1.838 \\ 1.824 \end{bmatrix} = \begin{bmatrix} 3.348 \\ 1.386 \\ 3.405 \end{bmatrix}$$

$$\mathbf{r}^{(2)} = \mathbf{r}^{(1)} - \alpha^{(1)} \mathbf{A} \mathbf{d}^{(2)} = \begin{bmatrix} 1.847 \\ 2.129 \\ 1.606 \end{bmatrix} - 1.388 \times \begin{bmatrix} 10 & -5 & -4 \\ -5 & 12 & -6 \\ -4 & -6 & 10 \end{bmatrix} \begin{bmatrix} 1.993 \\ 1.838 \\ 1.824 \end{bmatrix} = \begin{bmatrix} -2.923 \\ 0.532 \\ 2.658 \end{bmatrix}$$

$$i = 1 + 1 = 2$$

• With i=2 solve for $\beta^{(2)}$

$$\beta^{(2)} = \frac{\left[\mathbf{r}^{(2)}\right]^T \mathbf{r}^{(2)}}{\left[\mathbf{r}^{(1)}\right]^T \mathbf{r}^{(1)}} = \frac{15.897}{10.524} = 1.511$$

$$\mathbf{d}^{(2)} = \mathbf{r}^{(2)} + \boldsymbol{\beta}^{(2)} \mathbf{d}^{(1)} = \begin{bmatrix} -2.924 \\ 0.531 \\ 2.658 \end{bmatrix} + 1.511 \times \begin{bmatrix} 1.992 \\ 1.838 \\ 1.824 \end{bmatrix} = \begin{bmatrix} 0.086 \\ 3.308 \\ 5.413 \end{bmatrix}$$

Then

$$\alpha^{(2)} = \frac{(d^{(2)})' r^{(2)}}{(d^{(2)})' A d^{(2)}} = 0.078$$

And

$$\mathbf{x}^{(3)} = \mathbf{x}^{(2)} + \alpha^{(2)} \mathbf{d}^{(3)} = \begin{bmatrix} 3.348 \\ 1.386 \\ 3.405 \end{bmatrix} + 0.783 \times \begin{bmatrix} 0.086 \\ 3.308 \\ 5.413 \end{bmatrix} = \begin{bmatrix} 3.354 \\ 1.646 \\ 3.829 \end{bmatrix}$$

$$\mathbf{r}^{(3)} = \mathbf{r}^{(2)} - \alpha^{(2)} \mathbf{A} \mathbf{d}^{(3)} = \begin{bmatrix} -2.923 \\ 0.532 \\ 2.658 \end{bmatrix} - 0.783 \times \begin{bmatrix} 10 & -5 & -4 \\ -5 & 12 & -6 \\ -4 & -6 & 10 \end{bmatrix} \begin{bmatrix} 0.086 \\ 3.308 \\ 5.413 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$i = 2 + 1 = 3$$

Done in 3 = n iterations!

A comparison against Steepest Descent

iter	\mathbf{X}_1	\mathbf{X}_2	\mathbf{X}_3	\mathbf{r}_{1}	r_2	r_3	α		
0	0.000	0.000	0.000	10.000	-20.00	15.00	0.111		
1	0.582	-1.165	0.873	1.847	2.129	1.606	0.058		
2	2.487	1.030	2.530	0.398	-4.746	5.830	1.031		
3	2.511	0.745	2.880	0.135	0.892	0.717	0.060		
4	2.545	0.972	3.062	1.656	-0.565	0.392	0.254		
5	2.680	0.926	3.094	0.210	0.848	0.336	0.081		
Lots of iterations here									
68	3.352	1.644	3.827	0.002	-0.002	0.003	0.192		
69	3.353	1.644	3.827	0.001	0.002	0.001	0.078		
70	3.353	1.644	3.827	0.002	-0.001	0.003	0.192		
71	3.353	1.644	3.828	0.001	0.002	0.001	0.078		
72	3.353	1.644	3.828	0.002	-0.001	0.002	0.192		

In general SD need $O(\kappa(A))$ iterations where $O(\kappa(A))$ is the condition number of A while CG needs only the square root of this.

Preconditioned Conjugate Gradients

One problem is that the Conjugate Gradient method often fails on real problems. The solution is to use a preconditioner to transform the system to one that is more easily solved.

A simple approach uses $M^{-1}Ax = M^{-1}b$

Choices for Preconditioners

- Use Jacobi Method diagonal Matrix D as M inverse is straightforward
- Use Gauss Seidel Iteration

Pick
$$v_1$$

Let
$$r_1 = (b - Av_1)$$
 first residual $d_1 = M^{-1}r_1$ pick first direction

For
$$k = 1, 2, 3, n$$

 $q_k = Ad_k$

$$\alpha_k = \frac{r_k \cdot M^{-1} r_k}{d_k \cdot q_k}$$

$$v_{k+1} = v_k + \alpha_k d_k$$
 new value

$$\mathbf{r}_{k+1} = r_k - \alpha_k q_k$$
 new residual

$$\beta_k = \frac{r_{k+1}.M^{-1}r_{k+1}}{r_k.M^{-1}r_k}$$

$$d_{k+1} = M^{-1}r_{k+1} + \beta_k d_k$$
 new search direction

end

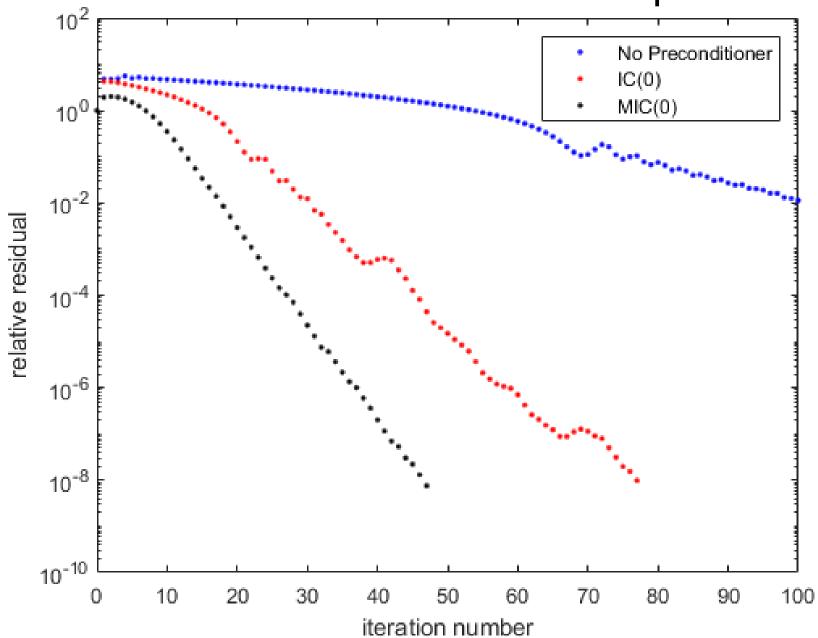
Preconditioned

Conjugate Gradient Algorithm

Note

One each step only need one new evaluation of M^{-1} to calculate $M^{-1}r_{k+1}$ which is saved for future steps

Effect of Preconditioners Matlab Example



Summary

Iterative methods when they work well may use many fewer floating point operations than direct methods and much less storage

Convergence is not assured and the methods may stall.

Solutions to this include preconditioners

Preconditioners may be very problem specific.

Nevertheless with the best iterative methods today we can solve very large systems on the largest parallel machines. Conjugate Gradient and gradient descent approaches are very important in data and AI applications.