

ME469A

Handout #8

Gianluca Iaccarino

Geometrical Example

Consider a two-equation system

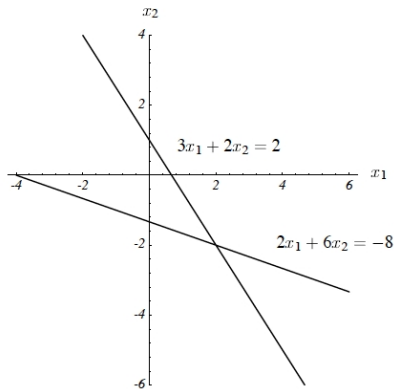
$$3x_1 + 2x_2 = 2$$

$$2x_1 + 6x_2 = -8$$

$$Ax = b$$

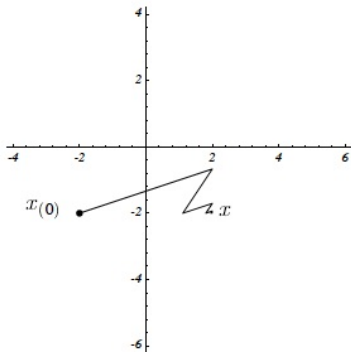
$$A = \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix}, b = \begin{pmatrix} 2 \\ -8 \end{pmatrix}$$

The solution is $x = [2, -2]^T$

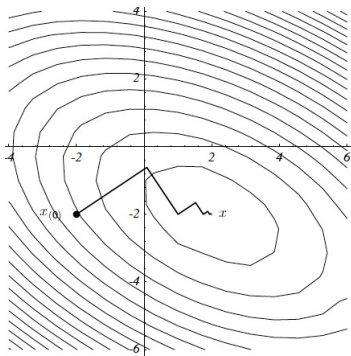


Convergence

- Basic (stationary) iterate is $Mx^{p+1} = Nx^p + b$
- Steepest descent iterate is $x^{p+1} = x^p + \alpha_p \rho_p$



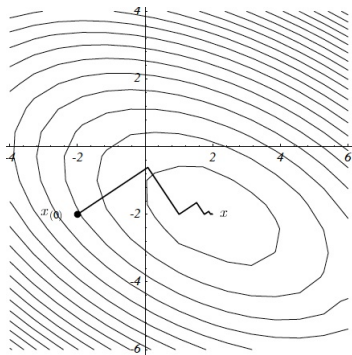
Jacobi



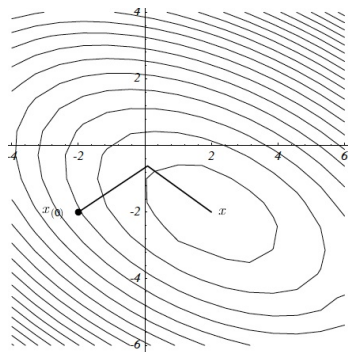
Steepest Descent

Convergence

- The idea of using minimization of the quadratic form to solve the problem can actually be useful...



Steepest Descent



Conjugate Gradient

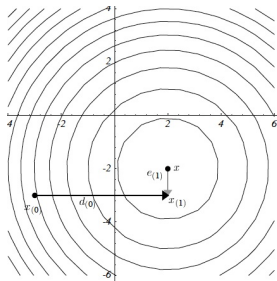
Generalized Descent Methods

- The extension consists in selecting **orthogonal** directions: never revisit the same direction

$$x^{p+1} = x^p + \alpha \rho_p \rightarrow x^{p+1} = x^p + \alpha d_p$$

- How do we build the d_p directions?
- d_p : one possible choice is the coordinate directions (x_1 and x_2)

Note: there are 2 dimensions, and therefore *only 2* orthogonal directions \rightarrow the method **should** converge in two steps



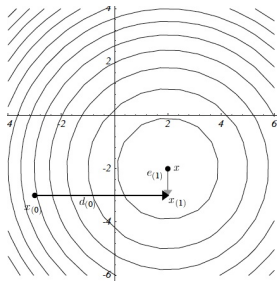
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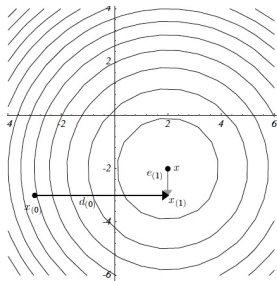
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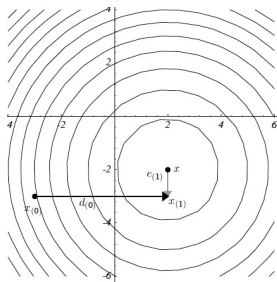
- $x^{p+1} = x^p + \alpha d_p$; we have d_p ,
how do we compute the α_p weight?
- in each direction, march enough to align the next guess with the exact solution, x

- Assume $d_0 = \rho_0$, and suppose you know ϵ_0, ϵ_1 .
- We could use the condition

$$(d_p^T \epsilon_{p+1}) = 0$$

$$(d_p^T (\epsilon_p + \alpha_p d_p)) = 0$$

$$\alpha_p = -\frac{d_p^T \epsilon_p}{d_p^T d_p}$$



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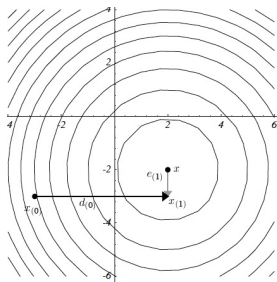
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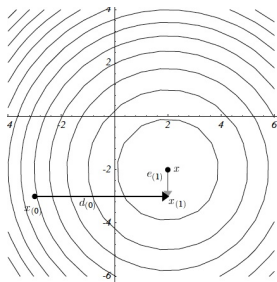
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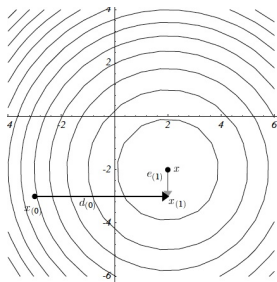
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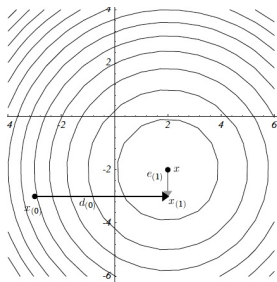
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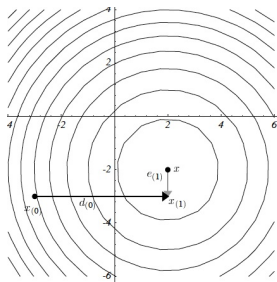
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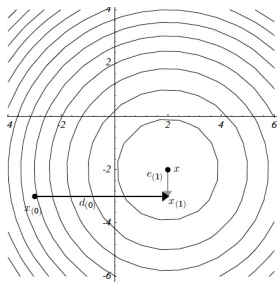
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$$x^{p+1} = x^p + \alpha d_p$$

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Descent Methods

- Steepest Descent

$$\rho_0 = b - Ax_0$$

do p=0...

$$\alpha_p = \frac{\rho_p^T \rho_p}{\rho_p^T (A \rho_p)}$$

$$x_{p+1} = x_p + \alpha_p \rho_p$$

$$\rho_{p+1} = \rho_p - \alpha_p (A \rho_p)$$

enddo

- Conjugate Gradient

$$\rho_0 = b - Ax_0 = d_0$$

do p=0...

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Descent Methods

- Steepest Descent

$$\rho_0 = b - Ax_0$$

do p=0...

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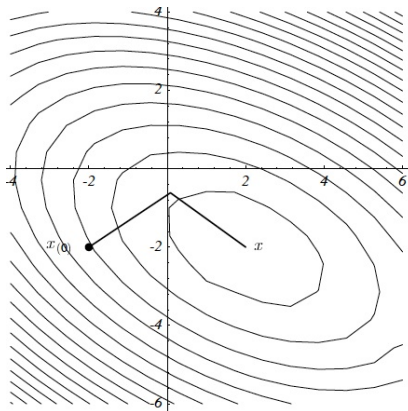
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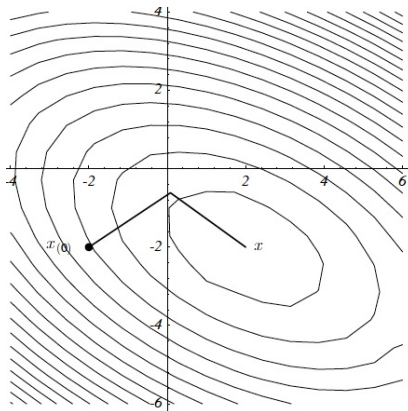
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- The convergence in 2 steps is **possible** but note that the directions d_p are NOT orthogonal, they are *A-orthogonal*

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Convergence comparisons

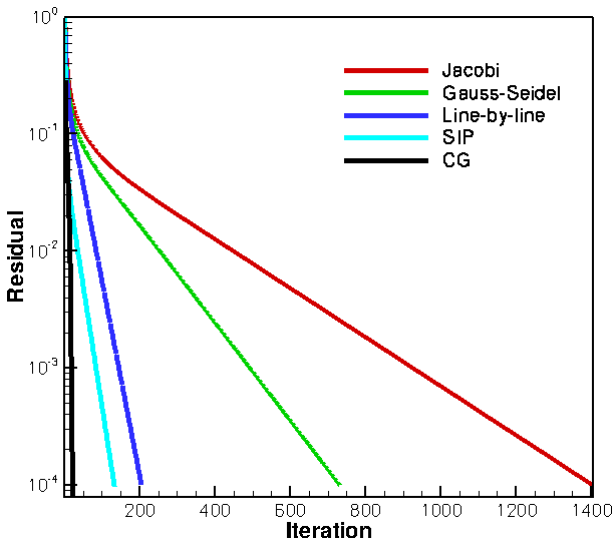
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- Code `lap12d.f`
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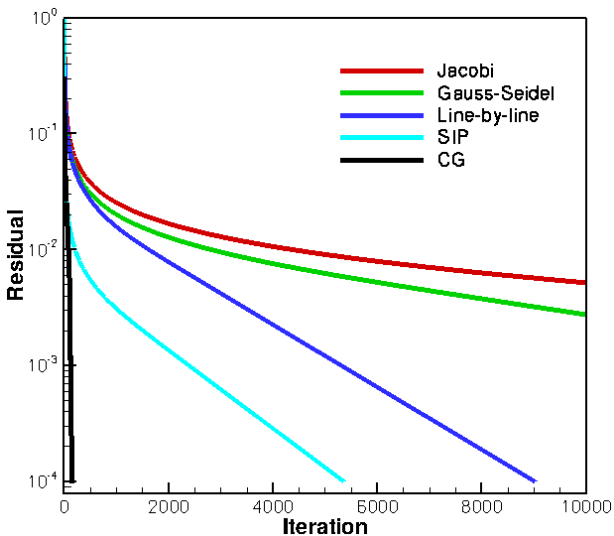
Convergence comparisons

Grid 32×32



Convergence comparisons

Grid 256×256



Convergence comparisons

- Convergence speed measured via **iteration count** strongly favors SIP and CG.
- This is not necessarily an useful measure, how about computational time?

	252×252	32×32
Jacobi	49.321	0.178
GS	45.583	0.111
LBL	69.698	0.087
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Convergence of descent methods

- The convergence of *classic* iterative methods (Jacobi, GS, etc.) is controlled by

$$e^{p+1} = (M^{-1}N)e^p$$

- The **convergence rate** $\omega = \|e^{p+1}\|/\|e^p\|$ is controlled by the spectral radius of $(M^{-1}N)$
- For descent methods it is possible to prove that $\omega = g(\kappa)$ where $\kappa = \lambda_{max}^A / \lambda_{min}^A$
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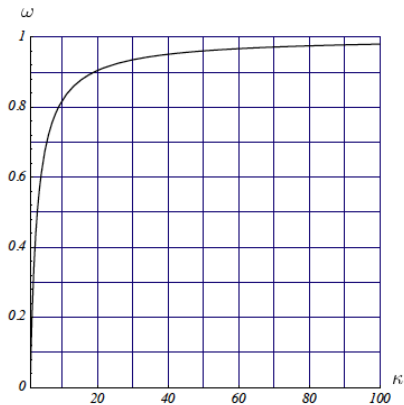
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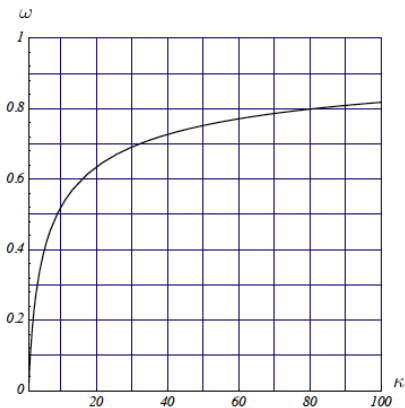
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Convergence rate

The relation $\omega = \omega(\kappa)$ can be determined theoretically



Steepest Descent



Conjugate Gradient

Preconditioning

- Preconditioning is a general technique for improving the condition number of a matrix
- The basic idea is that if we need to solve $Ax = b$ and assuming we have a matrix P whose inverse is easy to compute...
- we can solve the original problem by solving $P^{-1}Ax = P^{-1}b$
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Preconditioned Conjugate Gradient

- PCG is simple to implement and has good efficiency
- The cost is typically dominated by the matrix-vector multiplication
- The **preconditioner** used is typically $P = \text{diag}(A)$; other options are possible, the ILU(T) is typically one of the best choices
- The **nominal** convergence in $\text{size}(A)$ steps is never achieved because of **round-off** error
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Beyond structured grids

- The key element of CG-type solvers is the matrix-vector multiplication, e.g. compute a residual $\rho_p = b - A\phi^p$
- For a 5-point stencil (2D steady convection/diffusion or 2D Laplace) the matrix is pentadiagonal;

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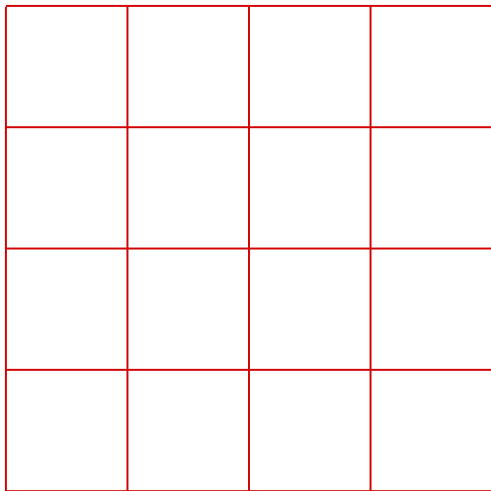
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Beyond structured grids

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			(4,4)
(1,2)			
(1,1)	(2,1)		

Beyond structured grids

Now it is really **unstructured**

			7
1	6		
4	12	14	

Beyond structured grids

- Never ever store A as $a_{ij} = [M][N]$
- For the **ordered** grid we build the matrix (row-by-row) assuming a **global CV index**

Matrix elements

```
for (int i=0; i<ni-1; i++) {  
  for (int j=0; j<nj-1; j++) {  
    int icv = i + (j-1)*ni // global index  
    ae[icv] = -(y[j]-y[j-1])/(xc[i+1]-xc[i])  
    aw[icv] = ...  
    as[icv] = ...  
    an[icv] = ...  
    ap[icv] = ...  
  }  
}
```

Residual evaluation

```
for (int icv=0; icv<(ni-1)*(nj-1); icv++) {  
  rho[icv] = q[icv] - as[icv]*phi[icv-ni]  
              - aw[icv]*phi[icv-1]  
              - an[icv]*phi[icv+ni]  
              - aw[icv]*phi[icv+1]  
              - ap[icv]*phi[icv]  
}
```

			(4.4)
(1.2)			
(1.1)	(2.1)		

Beyond structured grids

- Never ever store A as $a_{ij} = [M][N]$
- For the **ordered** grid we build the matrix (row-by-row) assuming a **global CV index**

Matrix elements

```
for (int i=0; i<ni-1; i++) {
  for (int j=0; j<nj-1; j++) {
    int icv = i + (j-1)*ni // global index
    ae[icv] = -(y[j]-y[j-1])/(xc[i+1]-xc[i])
    aw[icv] = ...
    as[icv] = ...
    an[icv] = ...
    ap[icv] = ...
  }
}
```

Residual evaluation

```
for (int icv=0; icv<(ni-1)*(nj-1); icv++) {
  rho[icv] = q[icv] - as[icv]*phi[icv-ni]
             - aw[icv]*phi[icv-1]
             - an[icv]*phi[icv+ni]
             - aw[icv]*phi[icv+1]
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```

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```

			(4,4)
(1,2)			
(1,1)	(2,1)		

Beyond structured grids

- For the **unstructured** grid we need more information
- We need to build a **list of neighbors** for each CV

			7
1	6		
4	12	14	

- One possibility is to have a list of **neighbors of CV**, `nbocv`
- `nbocv[0:15][0:3]` will do...BUT
- What about an unstructured grid with triangles? or polygons?
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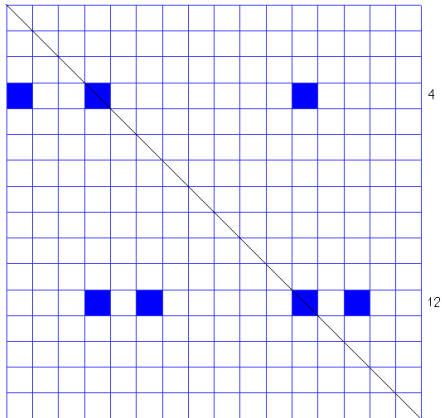
Beyond structured grids

- Sparse matrix for the unstructured ordering (the discretization is the same as before)

Matrix (16×16)

Grid ($N = 16$)

			7
1	6		
4	12	14	



General sparse matrices

- The idea is to **compress** all the non-zero matrix elements
- We store the matrix **row-by-row** as a sequence of entries skipping all the zeros - CRS structure (compressed row storage)

$$A = \begin{pmatrix} 10 & 0 & 0 & 0 & -2 & 0 \\ 3 & 9 & 0 & 0 & 0 & 3 \\ 0 & 7 & 8 & 7 & 0 & 0 \\ 3 & 0 & 8 & 7 & 5 & 0 \\ 0 & 8 & 0 & 9 & 9 & 13 \\ 0 & 4 & 0 & 0 & 2 & -1 \end{pmatrix}$$

val	10	-2	3	9	3	7	8	7	3...9	13	4	2	-1
col_ind	1	5	1	2	6	2	3	4	1...5	6	2	5	6
row_ptr	1	3	6	9	13	17	20						

- **val**: real array containing all the matrix entries $[0 : NZ - 1]$
- **col_ind**: the column index of the elements in **val** $[0 : NZ - 1]$
if $val(k) = a_{ij} \neq 0$ then $col_ind(k) = j$
- **row_ptr**: the location in **val** where a new row starts $[0 : M]$

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Matrix-Vector multiplication

CRS Format

Full Storage

$$A = \begin{pmatrix} 10 & 0 & 0 & 0 & -2 & 0 \\ 3 & 9 & 0 & 0 & 0 & 3 \\ 0 & 7 & 8 & 7 & 0 & 0 \\ 3 & 0 & 8 & 7 & 5 & 0 \\ 0 & 8 & 0 & 9 & 9 & 13 \\ 0 & 4 & 0 & 0 & 2 & -1 \end{pmatrix}$$

```
for (int icv = 0; icv < ncv; icv++) {
    y[icv] = 0;
    for (int jcv = 0; jcv < ncv; jcv++) {
        y[icv] += a[icv][jcv] * phi[jcv];
    }
}
```

val	10	-2	3	9	3	7	8	7	3...9	13	4	2	-1
col_ind	1	5	1	2	6	2	3	4	1...5	6	2	5	6
row_ptr	1	3	6	9	13	17	20						

```
for (int icv = 0; icv < ncv; icv++) {
    y[icv] = 0;
    int j_f = row_ptr[i];
    int j_l = row_ptr[i+1] - 1;
    for (int j = j_f; j <= j_l; j++)
        y[icv] += val[j] * phi[col_ind[j]];
}
```

Towards unstructured grids

The same **compressed** structure is used in handling unstructured grid connectivity

