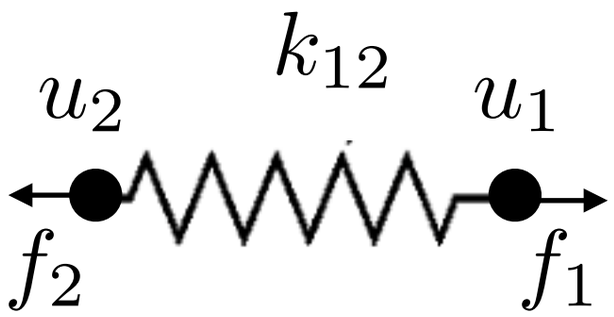
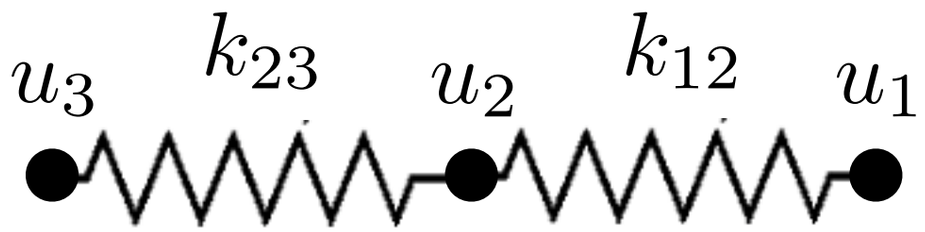
		授業計画	課題
04/06	第１回	微分方程式の離散化	前進・後退・中心差分，高次の差分を用いて 微分方程式を離散化し，誤差を評価できる
04/10	第２回	有限差分法	時間積分の安定性や高次精度の積分を理解し 移流・拡散・波動方程式を解析できる
04/13	第３回	有限要素法	Galerkin 法，テスト関数，isoparametric 要素 の概念を理解し，弾性方程式を解析できる
04/17	第４回	スペクトル法	Fourier・Chebyshev・Legendre・Bessel などの 直交基底関数による離散化の利点を説明できる
04/20	第５回	境界要素法	逆行列と δ 関数・Green 関数の関係を理解し 境界積分方程式を用いた解析ができる
04/24	第６回	分子動力学法	時間積分の symplectic 性や熱浴の概念を理解し 分子間に働く保存力の動力学を解析できる
04/27	第７回	Smooth particle hydrodynamics (SPH) 法	微分演算子の動径基底関数による離散化と その保存性・散逸性を評価できる
05/01	第８回	Particle mesh 法	粒子と格子の両方の離散化を組み合わせる場合の 離散点からの補間法と高次モーメントの保存法

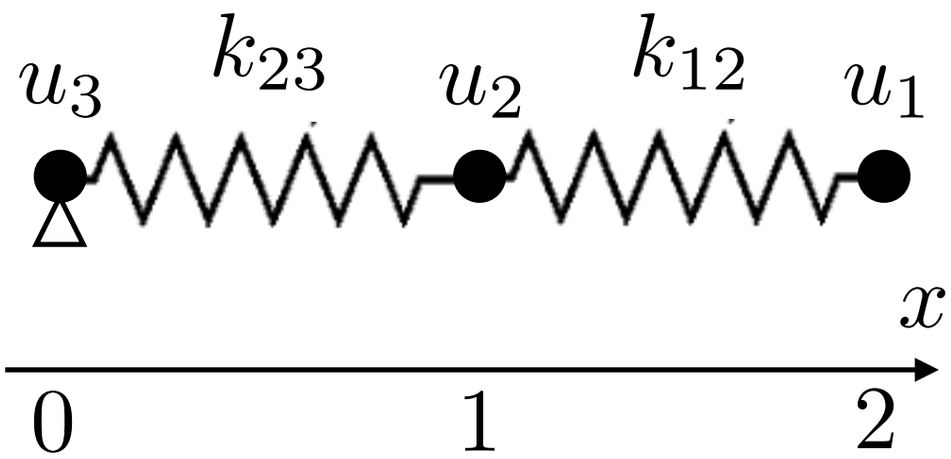
バネ



$$\begin{bmatrix} k_{12} & -k_{12} \\ -k_{12} & k_{12} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$$



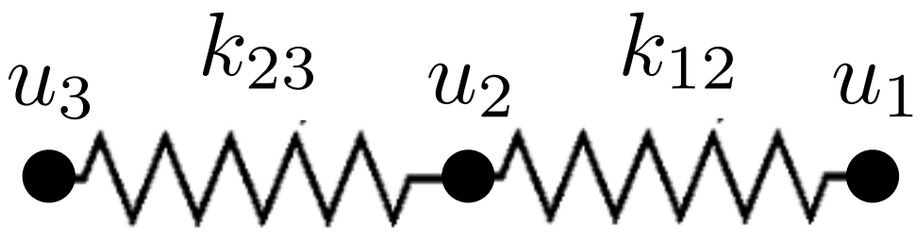
$$\begin{bmatrix} k_{12} & -k_{12} & 0 \\ -k_{12} & k_{12}+k_{23} & -k_{23} \\ 0 & -k_{23} & k_{23} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$



$$\begin{bmatrix} k_{12} & -k_{12} \\ -k_{12} & k_{12}+k_{23} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$$

$$-k_{23}u_2 = f_3$$

行列で表すと



$$K\ u = f$$

$$A = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix} \begin{matrix} k_{12} \\ k_{23} \end{matrix}$$
$$\begin{matrix} u_1 & u_2 & u_3 \end{matrix}$$

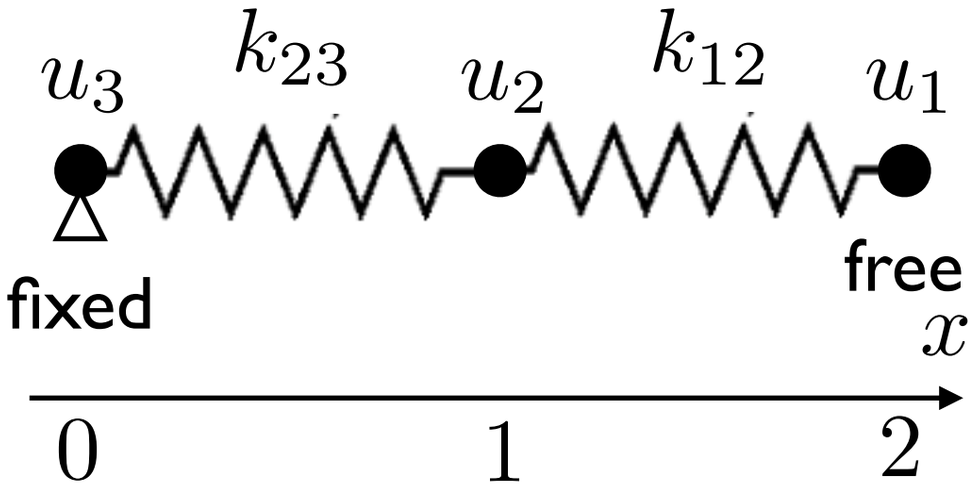
$$\begin{bmatrix} k_{12} & -k_{12} & 0 \\ -k_{12} & k_{12}+k_{23} & -k_{23} \\ 0 & -k_{23} & k_{23} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

$$A^T = \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{bmatrix}$$

$$C = \begin{bmatrix} k_{12} & 0 \\ 0 & k_{23} \end{bmatrix}$$

$$A^T C A = K$$

偏微分方程式で表すと



$$A^T C A u = f$$

$$-\frac{\partial}{\partial x}\left(c\frac{\partial u}{\partial x}\right) = f$$

$$A = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix}$$

u : displacement

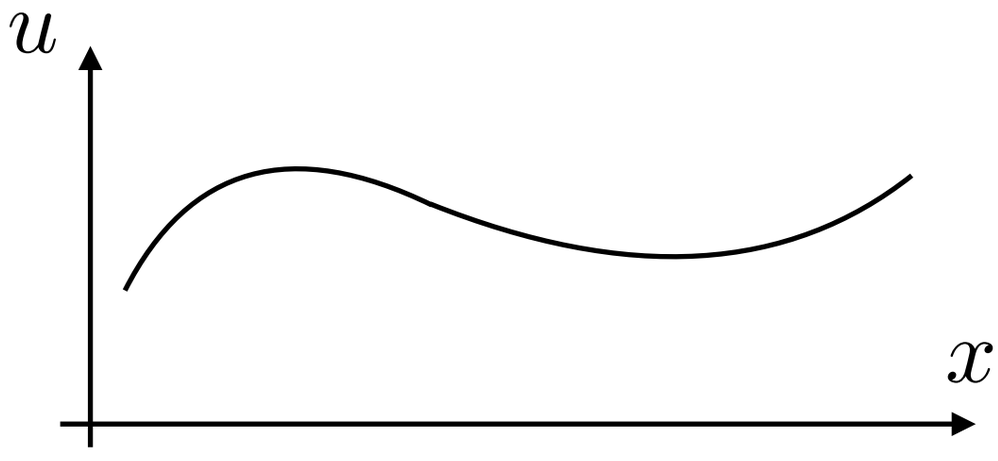
f : force

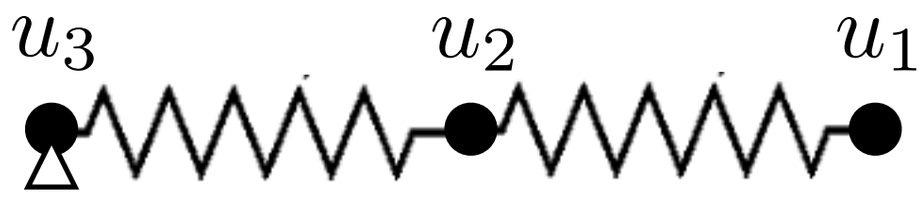
$$\epsilon = Au = \frac{\partial u}{\partial x} \longrightarrow \sigma = C\epsilon \longrightarrow f = A^T\sigma = -\frac{\partial \sigma}{\partial x}$$

ϵ : strain

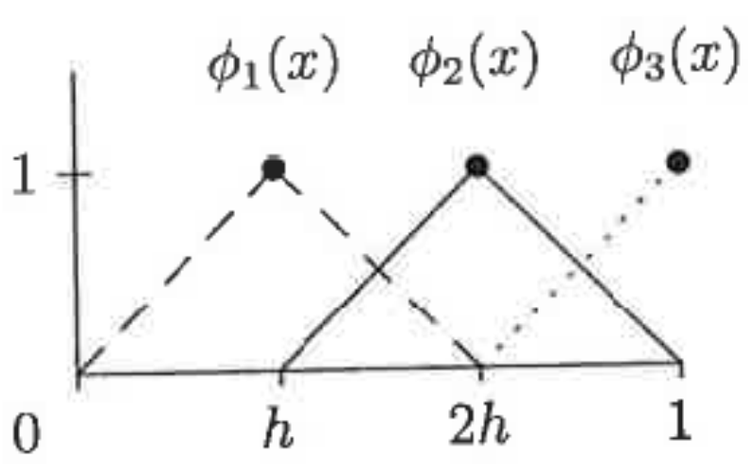
σ : internal stress

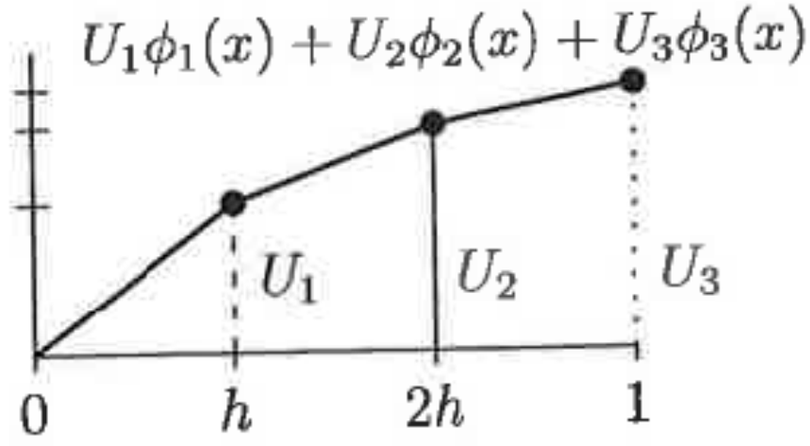
基底関数





$$u(x) = u_1\phi_1(x) + u_2\phi_2(x) + u_3\phi_3(x)$$

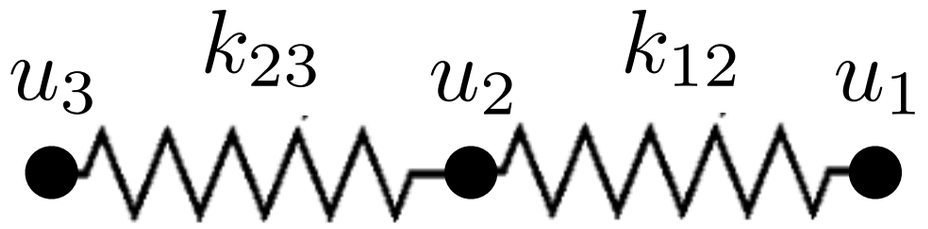


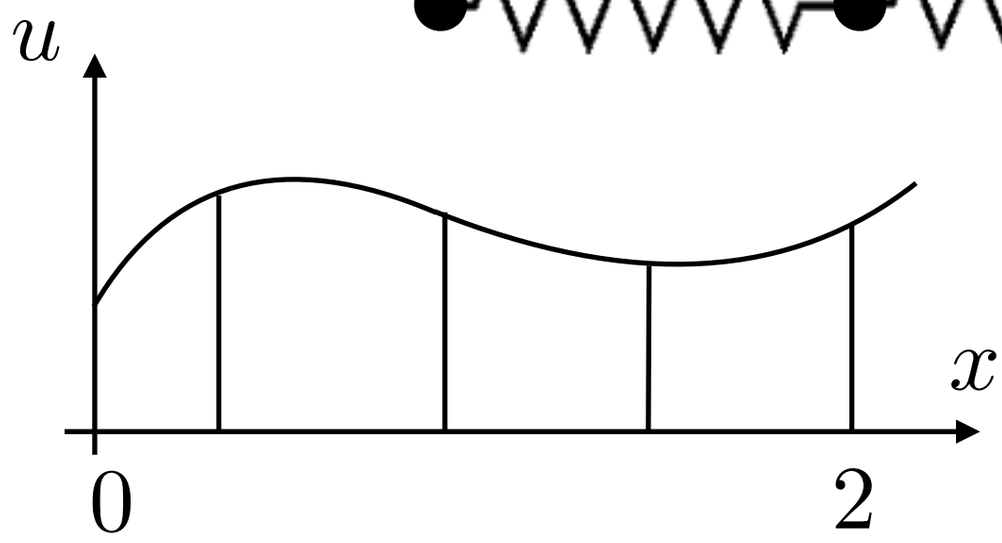


$$-\frac{\partial}{\partial x}\left(c\frac{\partial u}{\partial x}\right) = f \quad \longrightarrow \quad \sum_{i=1}^{3} -\frac{\partial}{\partial x}\left(c\frac{\partial \phi_i}{\partial x}\right) u_i = f$$

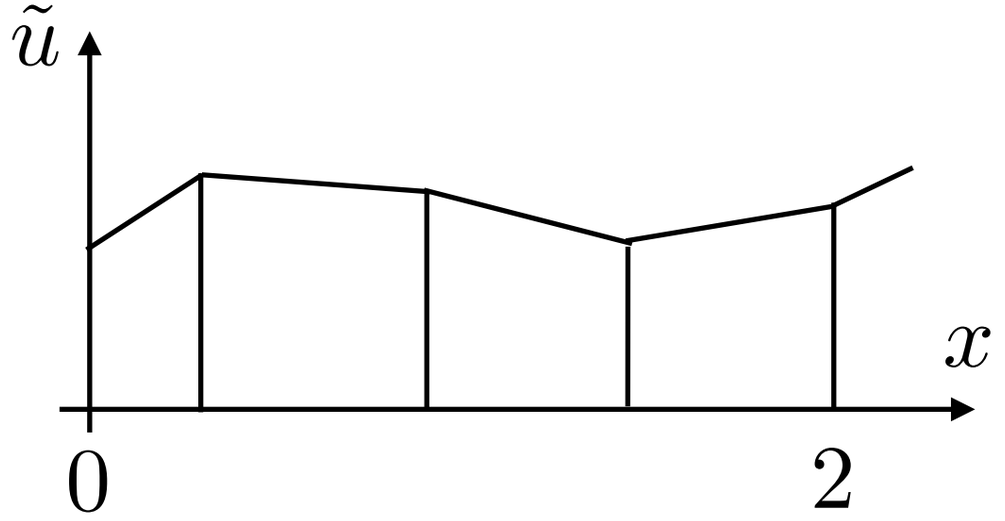
残差

$$-\frac{\partial}{\partial x}\left(c\frac{\partial u}{\partial x}\right) = f$$



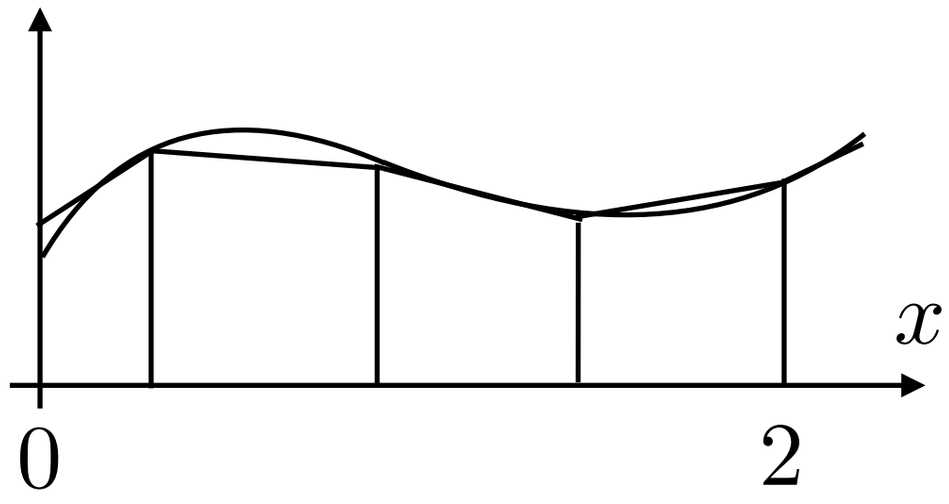


$$-\frac{\partial}{\partial x}\left(c\frac{\partial \tilde{u}}{\partial x}\right) \approx f$$



$$-\frac{\partial}{\partial x}\left(c\frac{\partial \tilde{u}}{\partial x}\right) - f = r$$

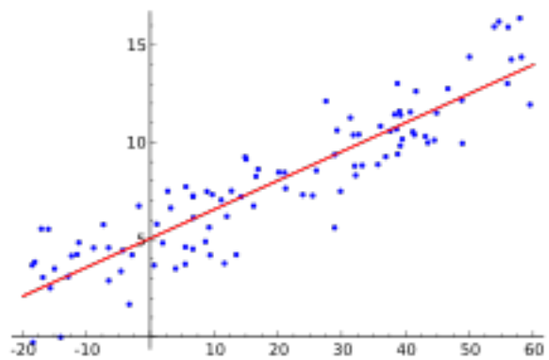
$$\int_0^2 r dx = 0$$



重み付き残差法

$$\int_0^2 rw = 0$$

Weighted residual



$$\int_0^2 r^2 = 0$$

Least squares

$$\int_0^2 r^2 w = 0$$

Weighted least squares

$$\int_0^2 \left(-\frac{\partial}{\partial x}\left(c\frac{\partial \tilde{u}}{\partial x}\right) - f \right) w dx = 0$$

$$\int_0^2 -\frac{\partial}{\partial x}\left(c\frac{\partial \tilde{u}}{\partial x}\right) w dx = \int_0^2 f w dx$$

部分積分→弱形式

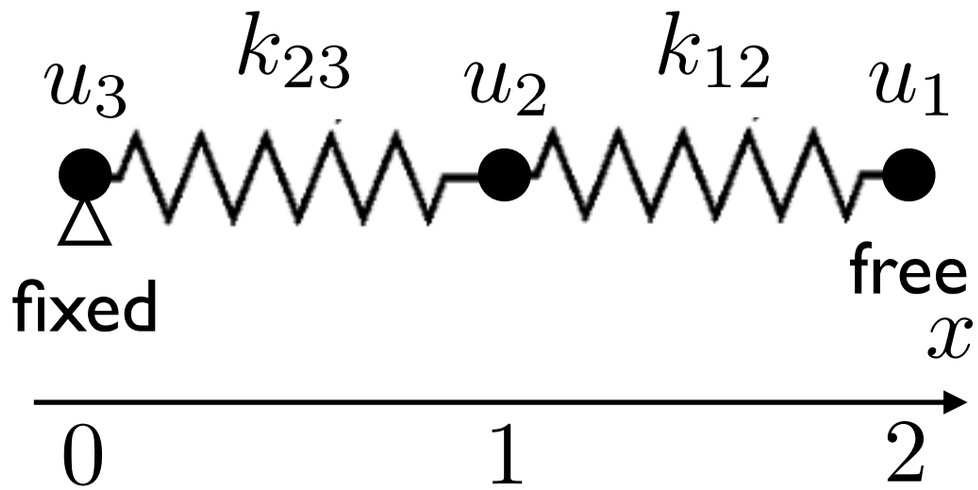
$$\int_0^2 -\frac{\partial}{\partial x}\left(c\frac{\partial \tilde{u}}{\partial x}\right) w dx = \int_0^2 f w dx$$

$$\int_0^2 -\frac{\partial}{\partial x}\left(c\frac{\partial \tilde{u}}{\partial x}\right) w dx = \int_0^2 c\frac{\partial \tilde{u}}{\partial x}\frac{\partial w}{\partial x} dx - \left[c\frac{\partial \tilde{u}}{\partial x} w\right]_0^2$$

境界条件

$$w(0) = 0$$

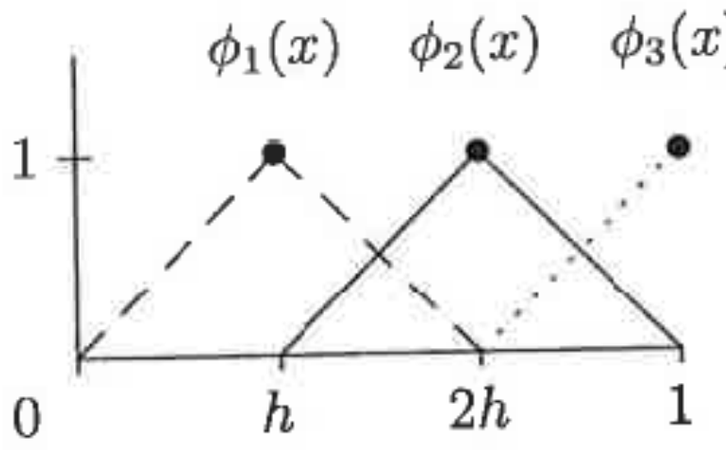
$$\frac{\partial \tilde{u}(2)}{\partial x} = 0$$

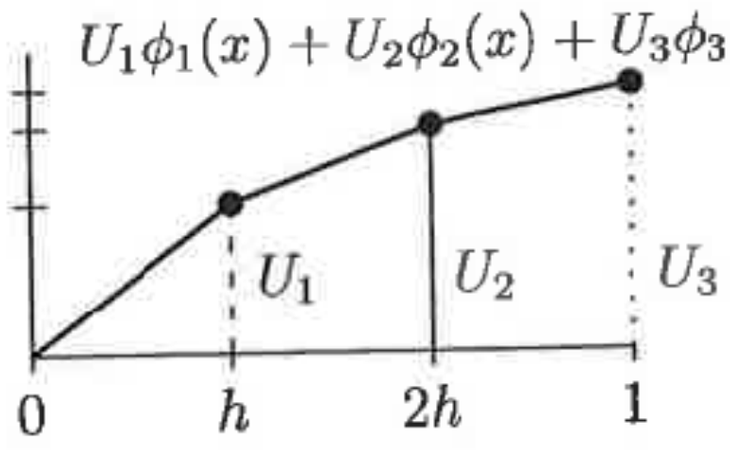


Galerkin 法

$$\int_0^2 c\frac{\partial \tilde{u}}{\partial x}\frac{\partial w}{\partial x}dx = \int_0^2 fwdx$$

$$w(x) = w_1\phi_1(x) + w_2\phi_2(x) + w_3\phi_3(x) \qquad w_1 = w_2 = w_3 = 1$$





$$w(x) = w_1(x) + w_2(x) + w_3(x)$$

$$\sum_{j=1}^{3}\int_0^2 c\frac{\partial \tilde{u}}{\partial x}\frac{\partial w_j}{\partial x}dx = \sum_{j=1}^{3}\int_0^2 fw_jdx$$

まとめると

$$\sum_{j=1}^{3}\int_0^2 c\frac{\partial \tilde{u}}{\partial x}\frac{\partial w_j}{\partial x}dx=\sum_{j=1}^{3}\int_0^2 f w_j dx \qquad \frac{\partial \tilde{u}}{\partial x}=\sum_{i=1}^{3}\frac{\partial \phi_i}{\partial x}u_i$$

$$\sum_{i,j=1}^{3}\int_0^2 c\frac{\partial \phi_i}{\partial x}\frac{\partial w_j}{\partial x}u_i dx=\sum_{j=1}^{3}\int_0^2 f w_j dx$$

$$K_{ij}=\int_0^2 c\frac{\partial \phi_i}{\partial x}\frac{\partial w_j}{\partial x} \qquad f_j=\int_0^2 f w_j dx$$

$$K\ u=f$$

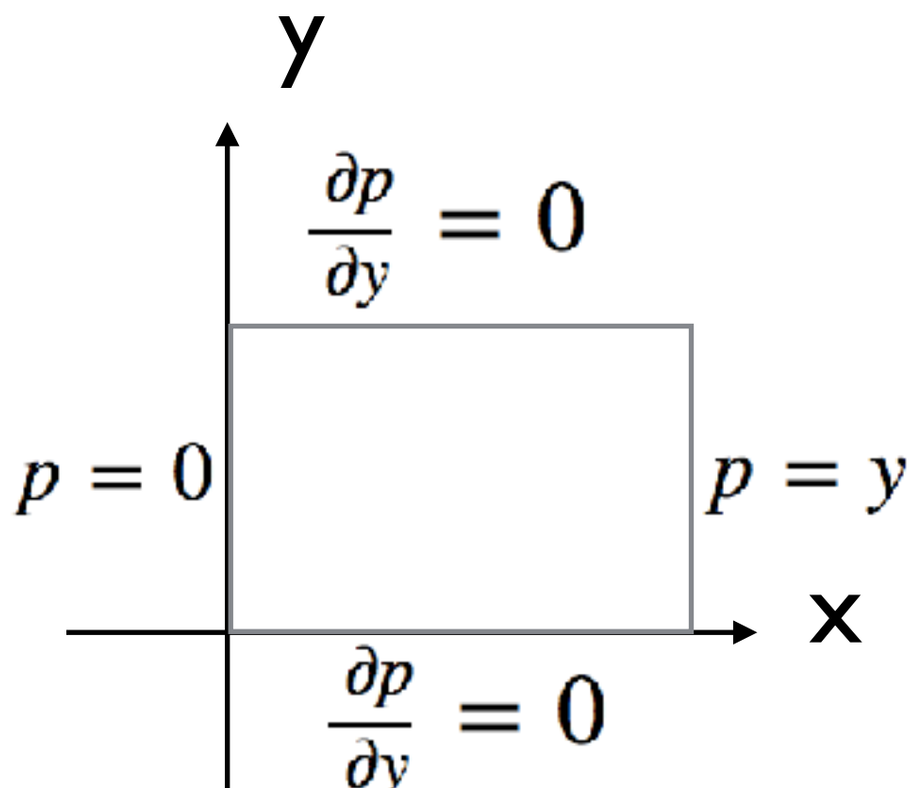
$$\begin{bmatrix} k_{12} & -k_{12} & 0 \\ -k_{12} & k_{12}+k_{23} & -k_{23} \\ 0 & -k_{23} & k_{23} \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}=\begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

		授業計画	課題
05/08	第９回	密行列の直接解法	LU 分解の原理を理解し，その最適化・並列化 と LINPACK ベンチマークの特徴を理解できる
05/11	第１０回	密行列の固有値解析	固有値・固有ベクトルの求め方を習得し対角化 正規直交化の高速化手法を理解できる
05/15	第１１回	疎行列の直接解法	AMD や Nested dissection などの並べ替え法と skyline・multifrontal 法の高速化手法を理解
05/18	第１２回	疎行列の反復解法	正定値行列や条件数の概念を理解し，Jacobi 法 CG 法，GMRES 法の相違点を理解
05/22	第１３回	反復法の前処理	前処理による条件数やスペクトル半径への影響や 前処理された CG 法の効果を理解できる
05/25	第１４回	マルチグリッド法	V-cycle における緩和・縮約・補間の役割を理解し 前処理法としての効果を理解できる
05/29	第１５回	FMM，H 行列	多重極展開，低ランク近似の概念を理解し 木構造の果たす役割を理解できる

2-D Laplace equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = 0$$

$$p_{i,j}^n = \frac{\Delta y^2 (p_{i+1,j}^n + p_{i-1,j}^n) + \Delta x^2 (p_{i,j+1}^n + p_{i,j-1}^n)}{2(\Delta x^2 + \Delta y^2)}$$



A=

$$\begin{bmatrix}
4 & -1 & & -1 & & & & & \\
-1 & 4 & -1 & & -1 & & & & \\
 & -1 & 4 & & & -1 & & & \\
-1 & & & 4 & -1 & & -1 & & \\
 & -1 & & -1 & 4 & -1 & & -1 & \\
 & & -1 & & -1 & 4 & & & -1 \\
 & & & -1 & & & 4 & -1 & \\
 & & & & -1 & & -1 & 4 & -1 \\
 & & & & & -1 & & -1 & 4
\end{bmatrix}$$

Ax=b

Sparse iterative solvers

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Sparse linear algebra (scipy.sparse.linalg)

Solving linear problems

Direct methods for linear equation systems:

spsolve(A, b[, permc_spec, use_umfpack])	Solve the sparse linear system Ax=b, where b may be a vector or a matrix.
factorized(A)	Return a fuction for solving a sparse linear system, with A pre-factorized.
MatrixRankWarning	
use_solver(**kwargs)	Select default sparse direct solver to be used.

Iterative methods for linear equation systems:

bicg(A, b[, x0, tol, maxiter, xtype, M, ...])	Use BIConjugate Gradient iteration to solve A x = b
bicgstab(A, b[, x0, tol, maxiter, xtype, M, ...])	Use BIConjugate Gradient STABilized iteration to solve A x = b
cg(A, b[, x0, tol, maxiter, xtype, M, callback])	Use Conjugate Gradient iteration to solve A x = b
cgs(A, b[, x0, tol, maxiter, xtype, M, callback])	Use Conjugate Gradient Squared iteration to solve A x = b
gmres(A, b[, x0, tol, restart, maxiter, ...])	Use Generalized Minimal RESidual iteration to solve A x = b.
lgmres(A, b[, x0, tol, maxiter, M, ...])	Solve a matrix equation using the LGMRES algorithm.
minres(A, b[, x0, shift, tol, maxiter, ...])	Use MINimum RESidual iteration to solve Ax=b
qmr(A, b[, x0, tol, maxiter, xtype, M1, M2, ...])	Use Quasi-Minimal Residual iteration to solve A x = b

Solvers

$$Ax = b$$

Dense matrix

Sparse matrix

Gauss Elimination

LU decomposition

Iterative solver

Direct solver

Multifrontal

Supernodal

Stationary method

Jacobi

Gauss-Seidel

SOR

Krylov subspace method

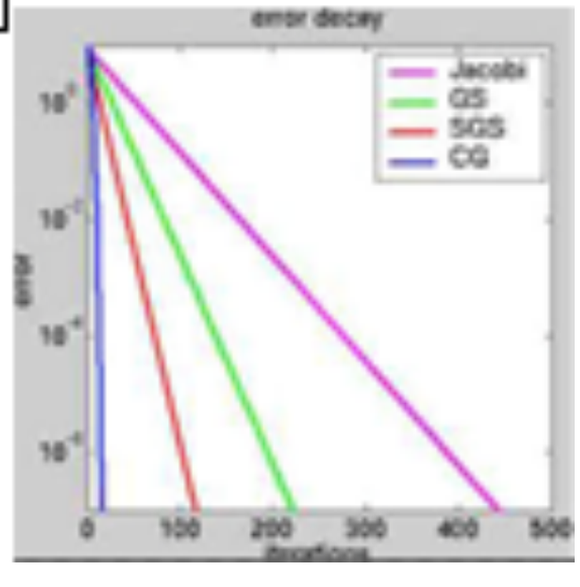
CG

BiCG

BiCGSTAB

GMRES

MINRES



Why iterative methods?

For many problems, it is not clear which method is best:

- Direct methods are robust
- $O(n^p)$ can have a very large constant for iterative methods
- Often a combination can be used, e.g. in domain decomposition or iterative refinement

Model problem	Direct	Iterative
Computational costs	$O(n^p)$ $p \approx 2.0$ for 2D $p \approx 2.3$ for 3D	$O(n^p)$ $p \approx 1.4$ for 2D $p \approx 1.2$ for 3D
Memory requirements	$O(n^p)$ $p \approx 1.5$ for 2D $p \approx 1.7$ for 3D	$O(n)$

Why iterative methods?

- Direct solvers are great for dense matrices and can be made to avoid roundoff errors to a large degree. They can also be implemented very well on modern machines.
- **Fill-in** is a major problem for certain sparse matrices and leads to extreme memory requirements (e.g., three-d.
- Some matrices appearing in practice are **too large** to even be represented explicitly (e.g., the Google matrix).
- Often linear systems only need to be **solved approximately**, for example, the linear system itself may be a linear approximation to a nonlinear problem.
- Direct solvers are much harder to implement and use on (massively) **parallel computers**.

Stationary Methods

Jacobi

$$x_i^{(k+1)} = x_i^k - \frac{1}{a_{ii}} \left(\sum_{j=1, j \neq i}^{n} a_{ij} \, x_j^{(k)} - b_i \right) \qquad i = 1, \ldots, n$$

Gauss-Seidel

$$x_i^{(k+1)} = x_i^k - \frac{1}{a_{ii}} \left(\sum_{j=1}^{i-1} a_{ij} \, x_j^{(k+1)} + \sum_{j=i+1}^{n} a_{ij} \, x_j^{(k)} - b_i \right) \qquad i = 1, \ldots, n$$

SOR

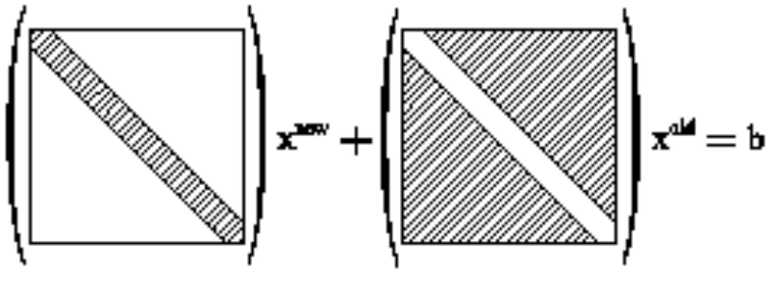
$$x_i^{(k+1)} = x_i^k - \frac{1}{a_{ii}} \omega \left(\sum_{j=1}^{i-1} a_{ij} \, x_j^{(k+1)} + \sum_{j=i+1}^{n} a_{ij} \, x_j^{(k)} - b_i \right) \qquad i = 1, \ldots, n$$

Stationary methods

$$\mathbf{A} = \mathbf{D} - \mathbf{L} - \mathbf{U}$$

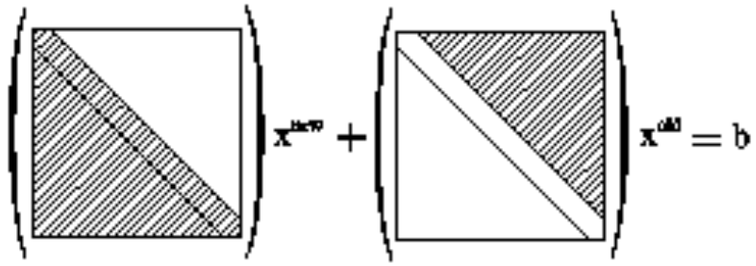
Jacobi Iteration

$$\mathbf{x}^{(k+1)} = \mathbf{D}^{-1}(\mathbf{L} + \mathbf{U})\mathbf{x}^{(k)} + \mathbf{D}^{-1}\mathbf{b}$$



Gauss-Seidel

$$\mathbf{x}^{(k+1)} = (\mathbf{I} - \mathbf{D}^{-1}\mathbf{L})^{-1}\mathbf{D}^{-1}\mathbf{U}\mathbf{x}^{(k)} + (\mathbf{I} - \mathbf{D}^{-1}\mathbf{L})^{-1}\mathbf{D}^{-1}\mathbf{b}$$



Successive Over-Relaxation

$$\mathbf{x}^{(k+1)} = (\mathbf{D} - \omega\mathbf{L})^{-1}((1-\omega)\mathbf{D} + \omega\mathbf{U})\mathbf{x}^{(k)} + (\mathbf{D} - \omega\mathbf{L})^{-1}\omega\mathbf{b}$$

Basic Iterative Methods for Linear Systems

Consider the system of equations

$$Ax = b.$$

Let us split A into

$$A = M - K$$

where M is any non-singular matrix and $K = M - A$.
Hence, $Ax = b$ becomes

$$\begin{aligned}(M - K)x &= b \\ Mx &= Kx + b \\ x &= M^{-1}Kx + M^{-1}b\end{aligned}$$

Basic Iterative Methods for Linear Systems, cont'd

This suggests the iteration scheme: For $k = 1, 2, 3, \ldots$ repeat

$$x^{(k+1)} = M^{-1}Kx^{(k)} + M^{-1}b$$

until convergence.

Of course, for this iteration to be computationally practical, the splitting of A should be chosen such that $M^{-1}K$ and $M^{-1}b$ are easy to calculate.

We will study splittings based on the diagonal, and the upper / lower triangular parts of A:

$$A = D - U - L$$

Jacobi's Method

So-called Jacobi iteration is defined by choosing the splitting

$$A = D - (L + U) = M - K$$

where D is the diagonal of A, $-L$ is the strictly lower triangle of A, and $-U$ is the strictly upper triangle of A.

The iteration scheme takes the form

$$x^{(k+1)} = D^{-1}(L + U)x^{(k)} + D^{-1}b$$

Note that D is easy to invert since it is a diagonal matrix.

The Gauss-Seidel Method

In the (forward) Gauss-Seidel method A is split into

$$A = (D - L) - U = M - K$$

yielding the iteration scheme

$$x^{(k+1)} = (D - L)^{-1}(Ux^{(k)} + b)$$

Since $D - L$ is lower triangular the effect of $(D - L)^{-1}$ can be computed by forward elimination.

The (backward) Gauss-Seidel method instead uses

$$A = (D - U) - L = M - K$$

Successive Over-Relaxation (SOR)

A more sophisticated method is obtained by choosing

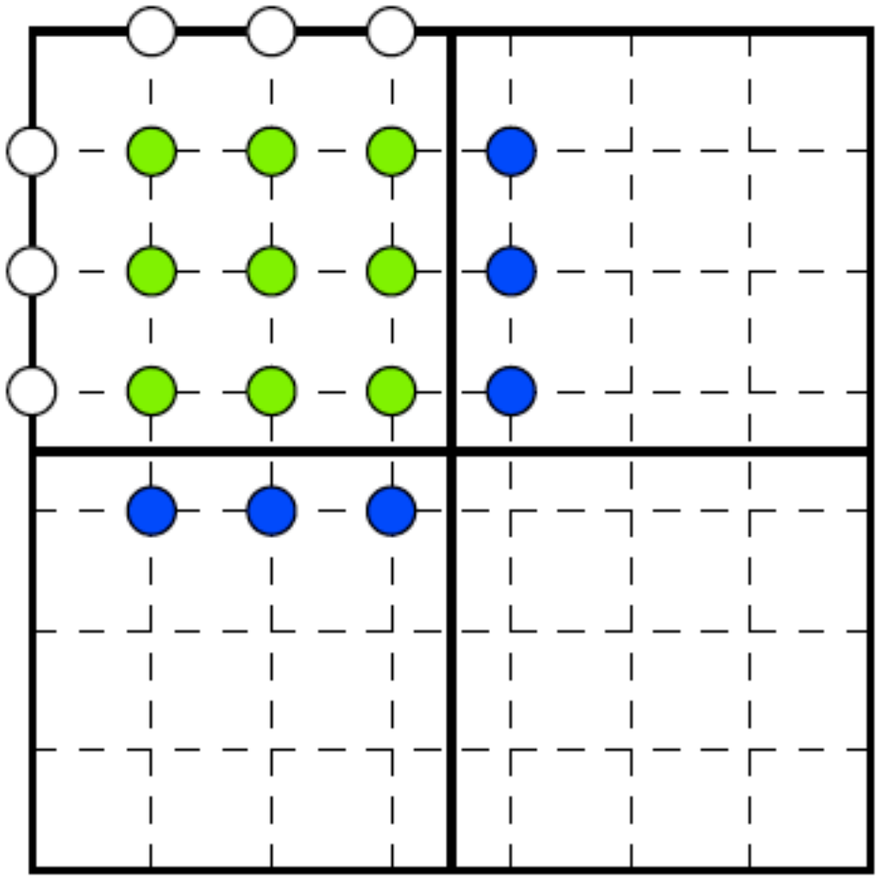
$$A = (\frac{1}{\omega}D - L) - (\frac{1-\omega}{\omega}D + U) = M - K$$

where ω is a relaxation parameter.

This gives the iteration scheme

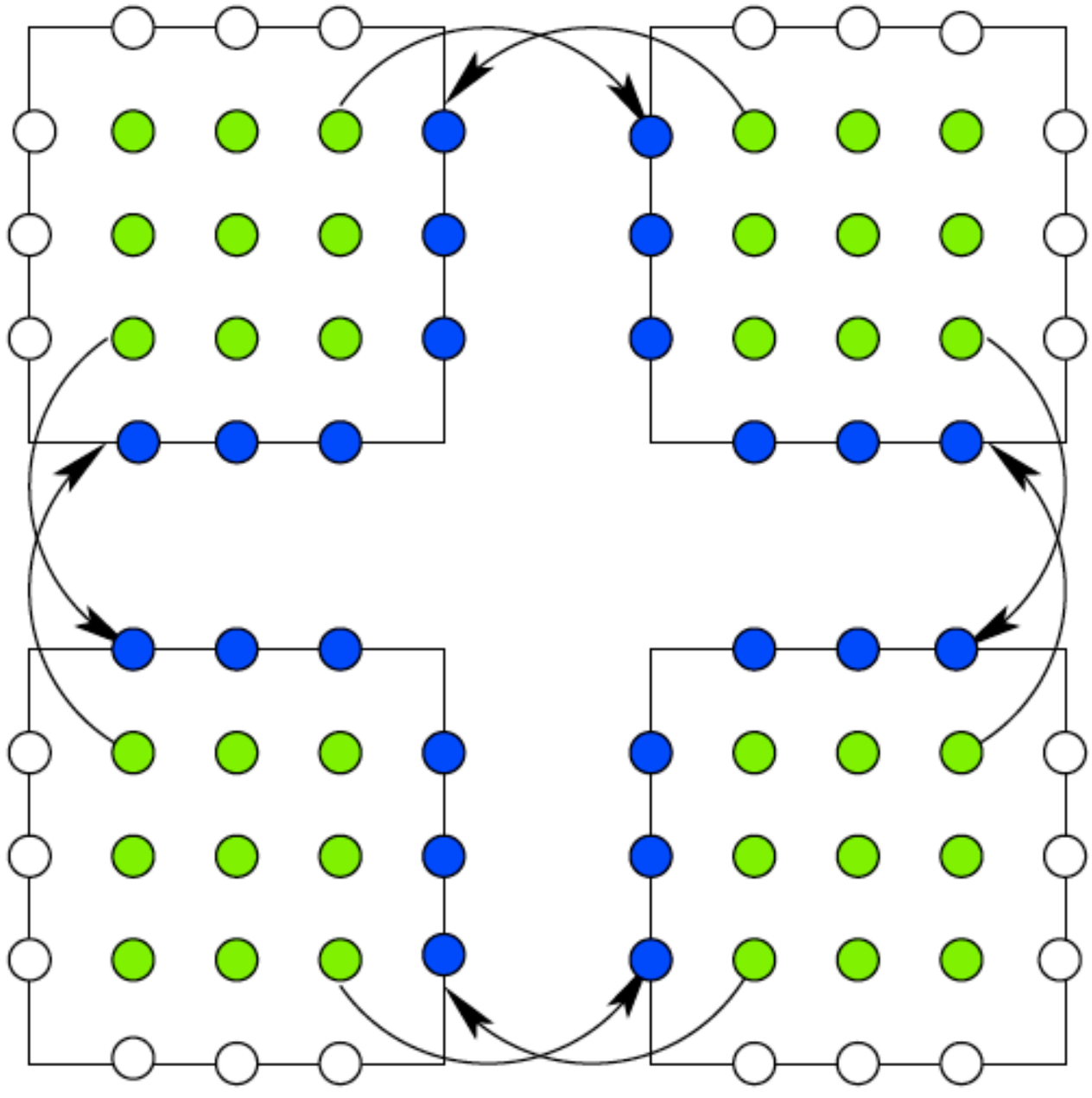
$$x^{(k+1)} = (D - \omega L)^{-1}(\omega U + (1-\omega)D)x^{(k)} + \omega(D - \omega L)^{-1}b$$

Parallel version (5 point stencil)



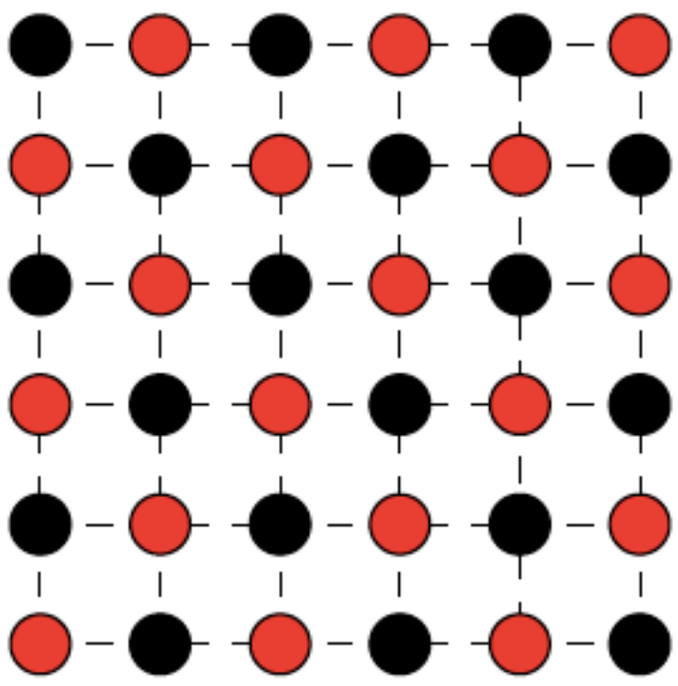
Boundary values: white
Data on P0: green
Ghost cell data: blue

Parallel version (5 point stencil)



Communicate ghost cells before each step.

Red-Black Gauss-Seidel



Red depends only on black, and vice-versa.
Generalization: multi-color orderings

Red black Gauss-Seidel step

```
for i = 2:n-1
  for j = 2:n-1
    if mod(i+j,2) == 0
      u(i,j) = ...
    end
  end
end

for i = 2:n-1
  for j = 2:n-1
    if mod(i+j,2) == 1,
    u(i,j) = ...
  end
end
```

Solvers

$$Ax = b$$

Dense matrix

Sparse matrix

Gauss Elimination

LU decomposition

Iterative solver

Direct solver

Multifrontal

Supernodal

Stationary method

Jacobi

Gauss-Seidel

SOR

Krylov subspace method

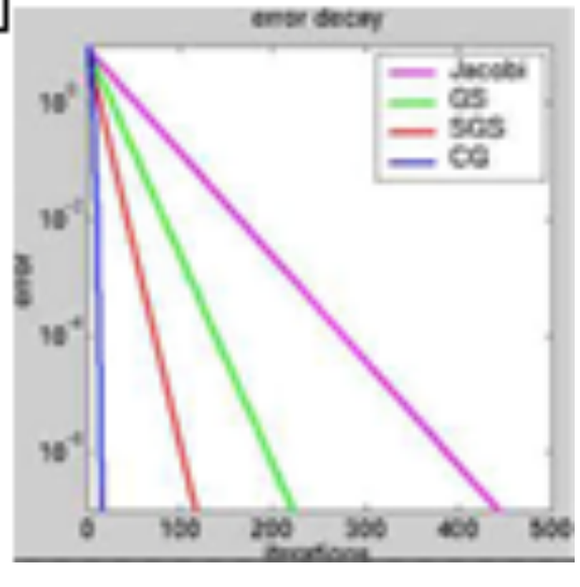
CG

BiCG

BiCGSTAB

GMRES

MINRES



Alexei Nikolaevich Krylov

1863-1945

Maritime Engineer

300 papers and books:
shipbuilding, magnetism,
artillery, math, astronomy

1890: Theory of oscillating
motions of the ship

1931: *Krylov subspace methods*

Conjugate gradient method as iterative method

in exact arithmetic

- CG was originally proposed as a direct (non-iterative) method
- in theory, convergence in at most n steps

in practice

- due to rounding errors, CG method can take $\gg n$ steps (or fail)
- CG is now used as an iterative method
- with luck (good spectrum of A), good approximation in $\ll n$ steps
- attractive if matrix-vector products are inexpensive

conjugate gradient

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In mathematics, the **conjugate gradient** method is an algorithm for the numerical solution of particular systems of linear equations, namely those whose matrix is symmetric and positive-definite.

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In mathematics, the **conjugate gradient** method is an algorithm for the numerical solution of particular systems of linear equations, namely those whose matrix is symmetric and positive-definite.
Nonlinear conjugate gradient - Preconditioner - Biconjugate gradient method

[PDF] An Introduction to the Conjugate Gradient Method Without...
www.cs.cmu.edu/~quake-papers/painless-**conjugate-gradient**.pdf
by JR Shewchuk - 1994 - Cited by 1646 - Related articles
The idea of quadratic forms is introduced and used to derive the methods of Steepest Descent, **Conjugate** Directions, and **Conjugate Gradients**. Eigenvectors are explained and used to examine the convergence of the Jacobi Method, Steepest Descent, and **Conjugate Gradients**.

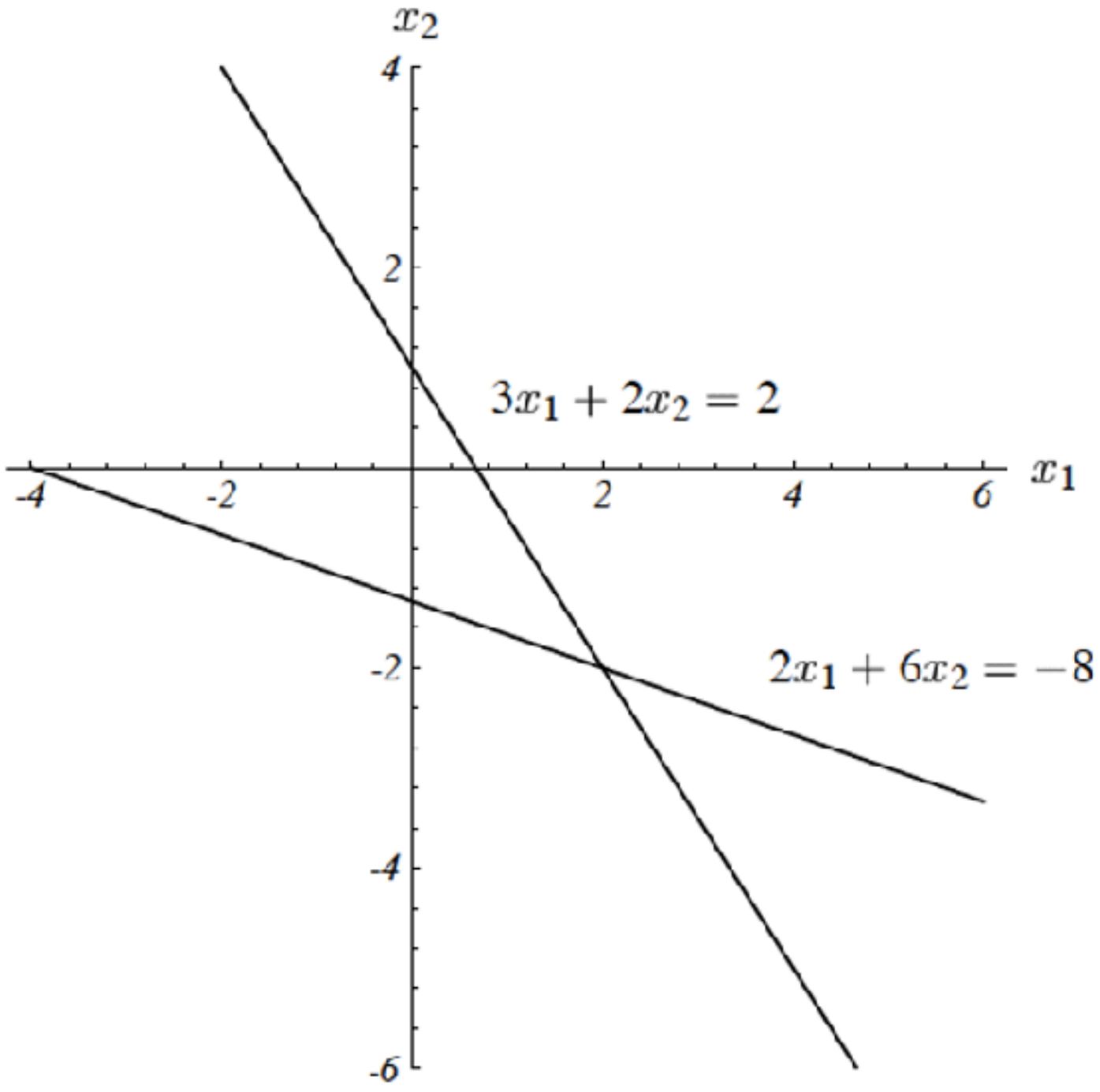
An Introduction to the Conjugate Gradient Method Without the Agonizing Pain

Edition $1\frac{1}{4}$

Jonathan Richard Shewchuk

August 4, 1994

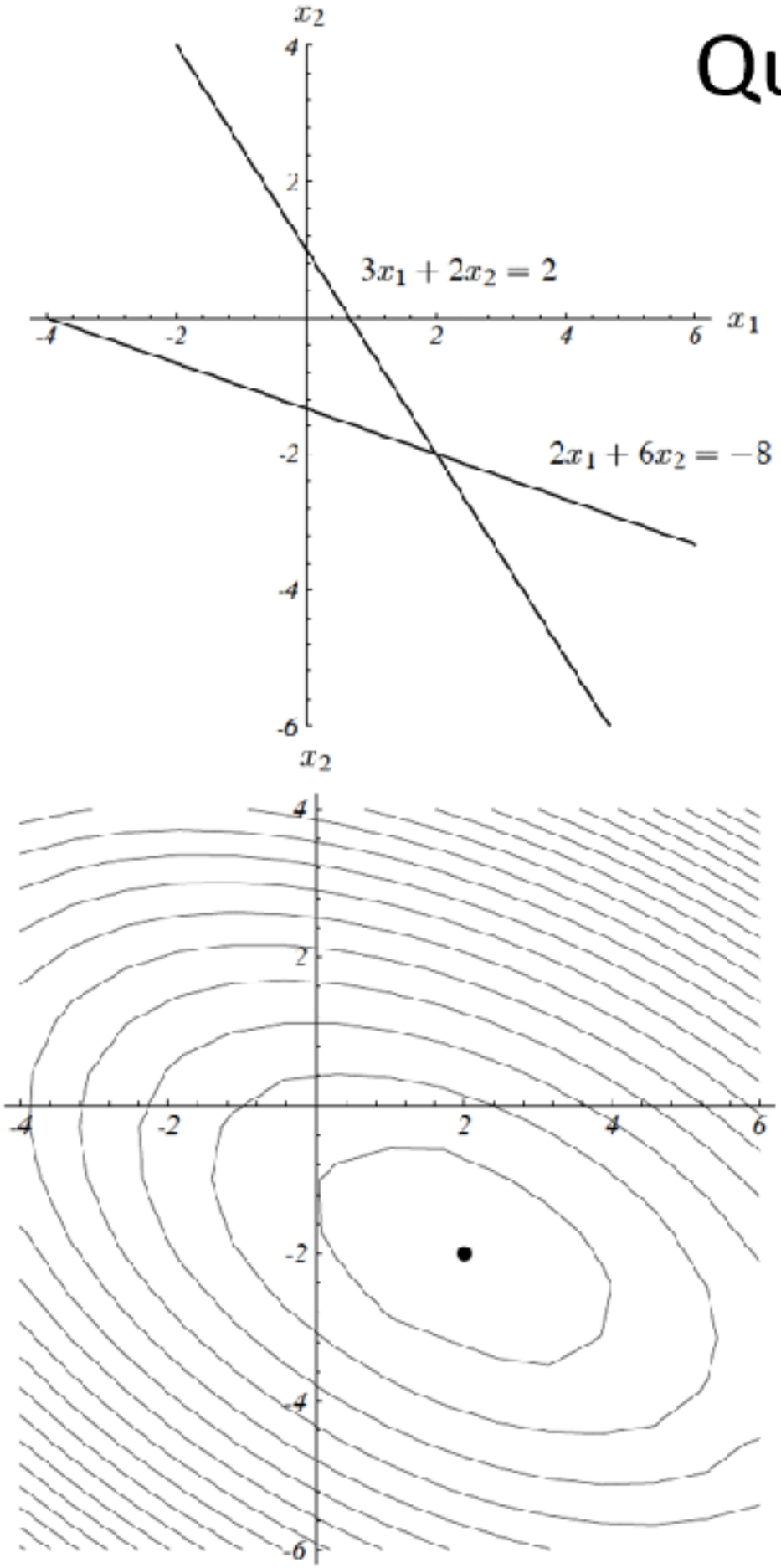
2x2 example



$$Ax = b$$

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

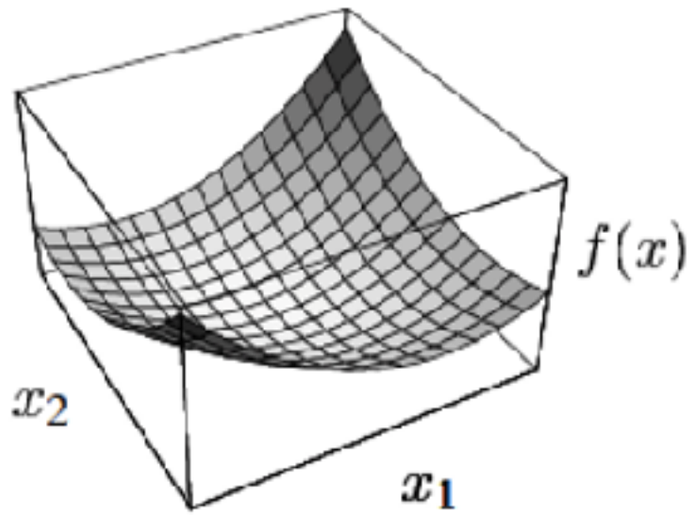
Quadratic function



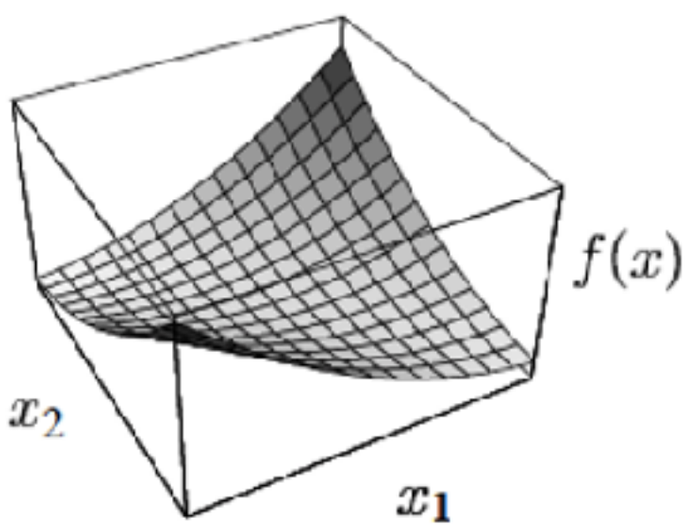
$$f(x) = \frac{1}{2}x^T Ax - b^T x$$

$$f'(x) = Ax - b.$$

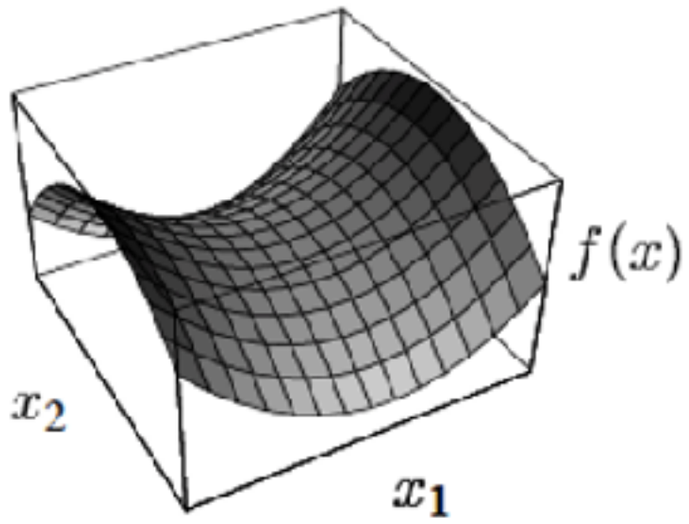
Positive definite $x^T Ax > 0$



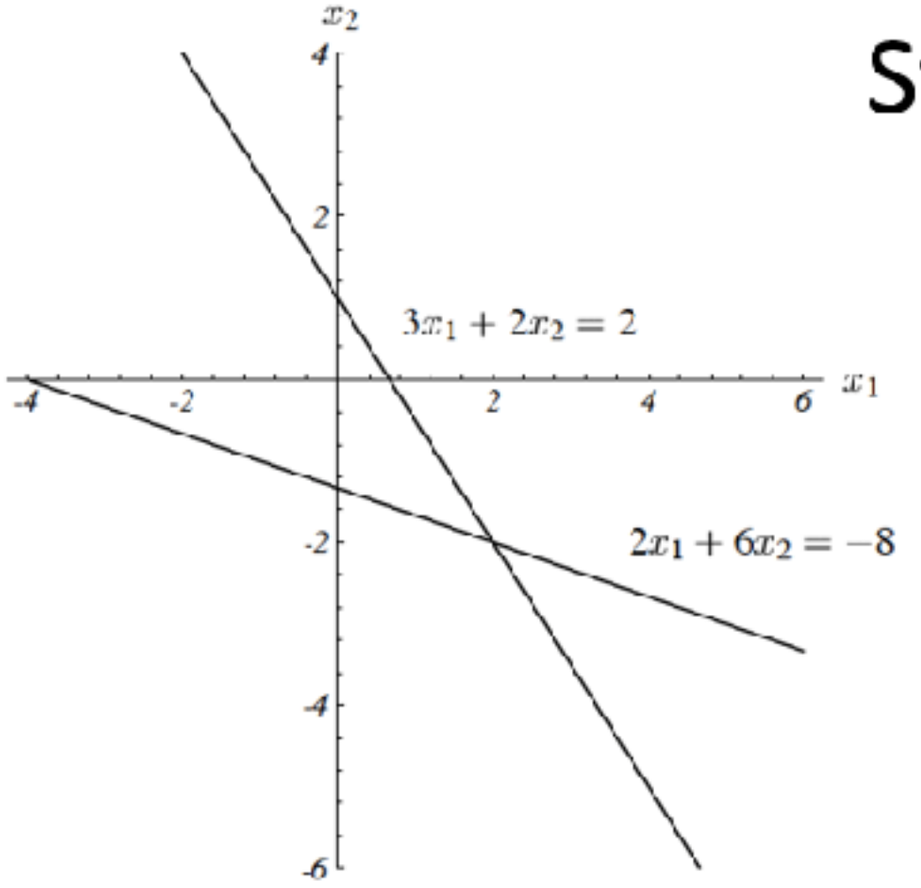
Singular



Indefinite

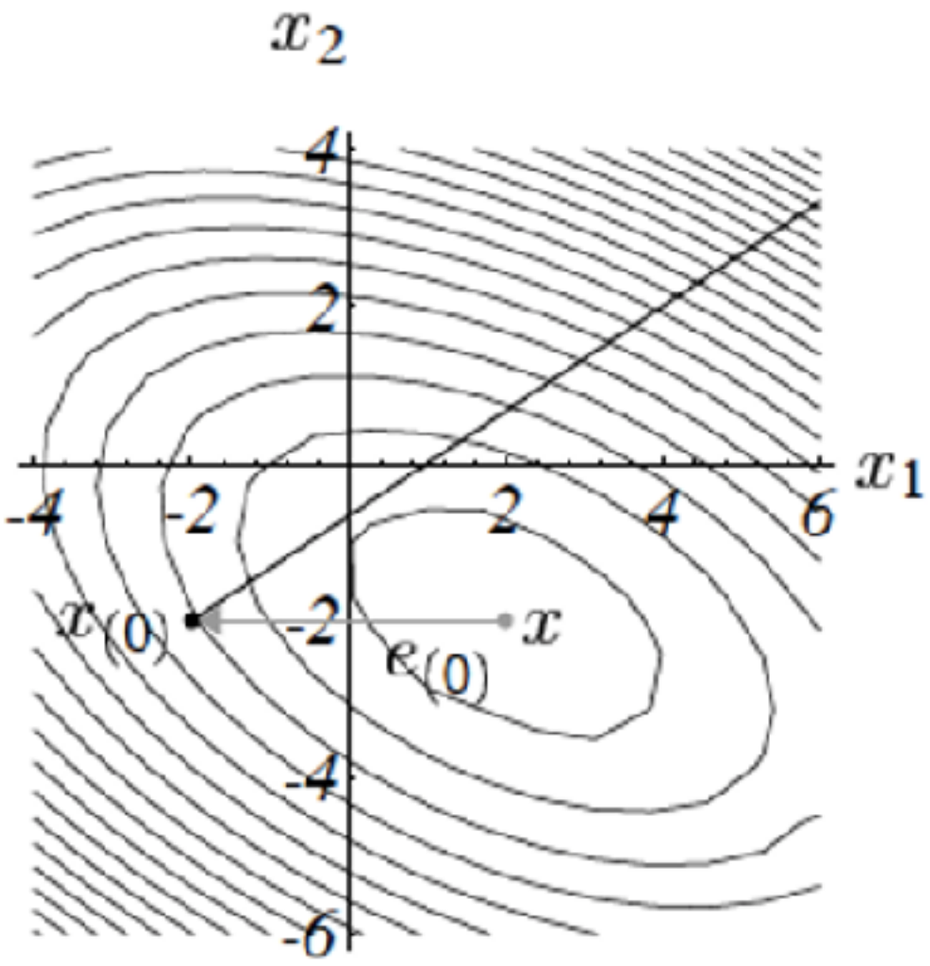


Steepest decent



$$e_{(i)} = x_{(i)} - x$$

$$r_{(i)} = b - Ax_{(i)} = -Ae_{(i)} = -f'(x_{(i)})$$



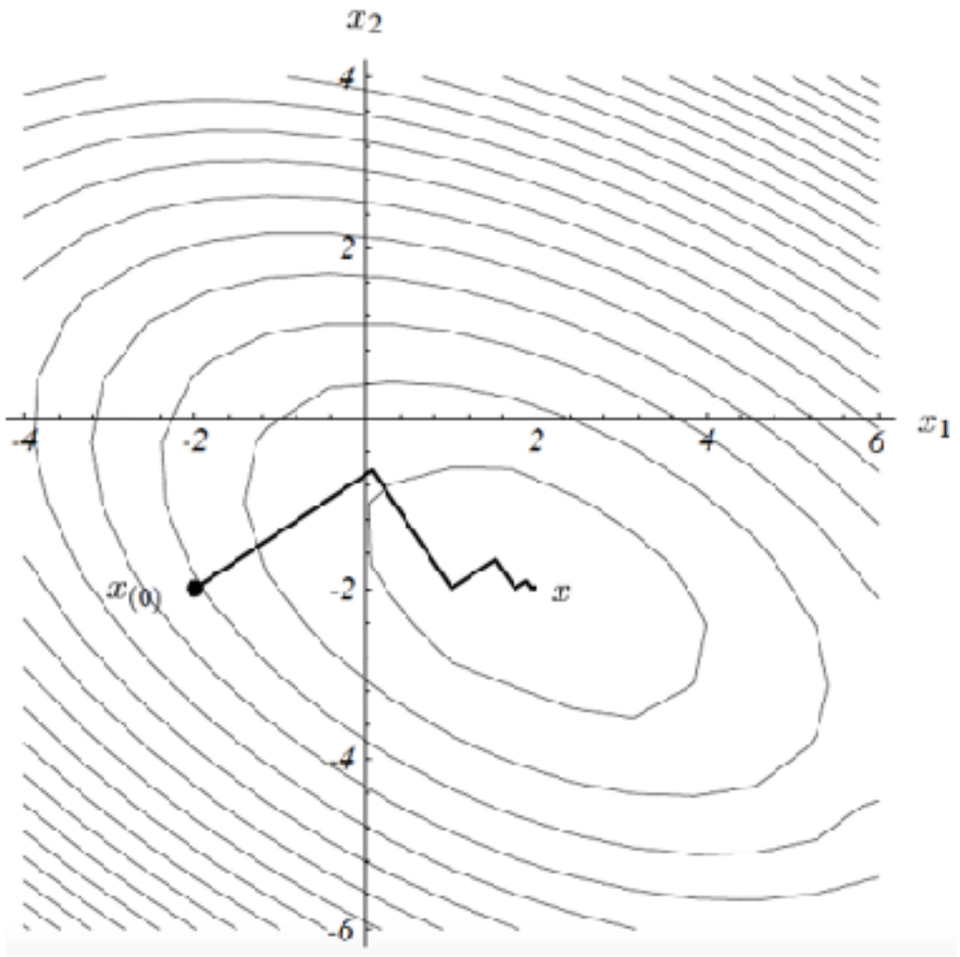
Suppose we start at $x_{(0)} = [-2, -2]^T$

We take a series of steps $x_{(1)}, x_{(2)}, \ldots$

$$x_{(1)} = x_{(0)} + \alpha r_{(0)}$$

$$r_{(1)}^T r_{(0)} = 0$$

Steepest decent



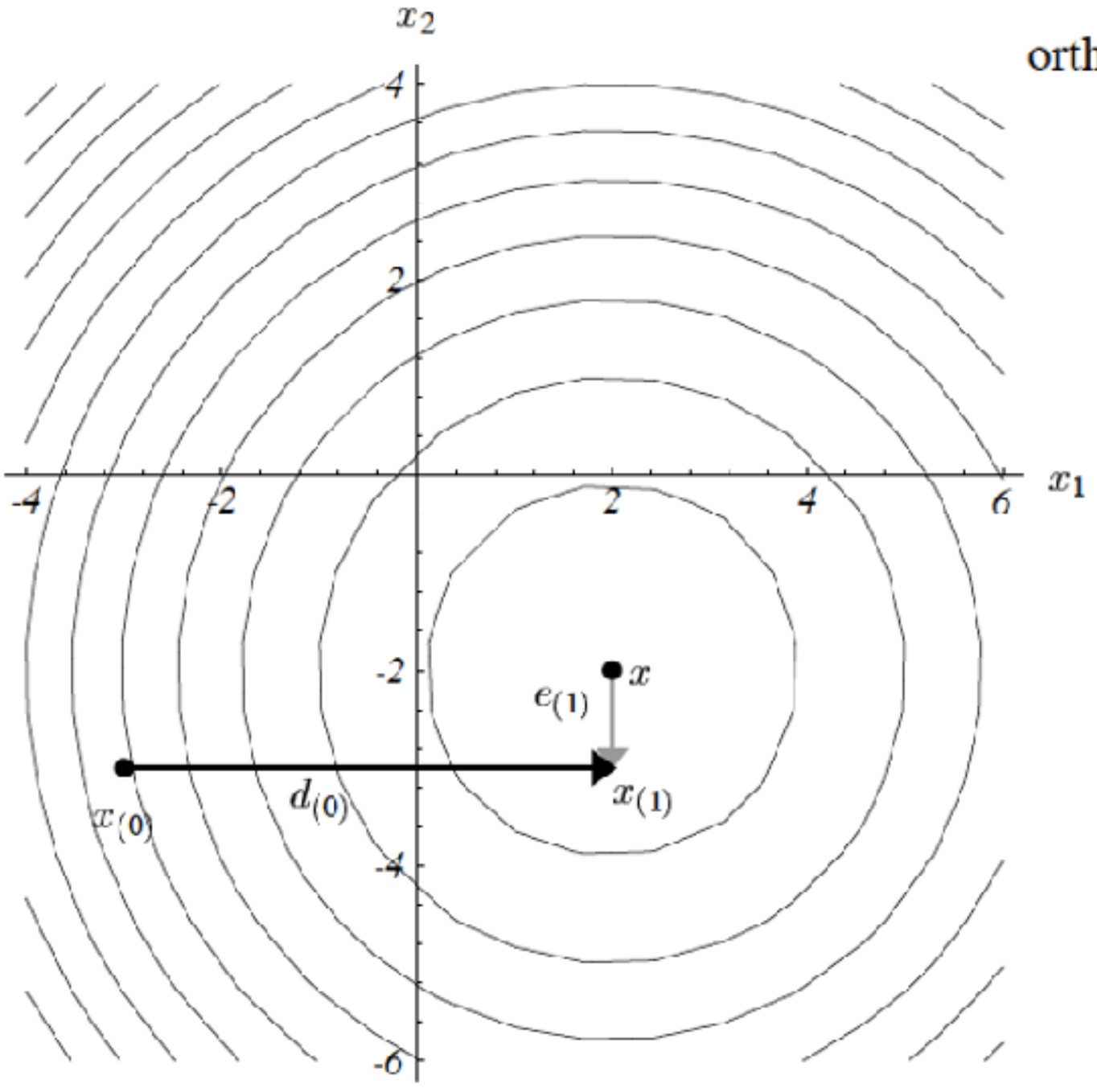
$$
\begin{aligned}
r_{(1)}^T r_{(0)} &= 0 \\
(b - Ax_{(1)})^T r_{(0)} &= 0 \\
(b - A(x_{(0)} + \alpha r_{(0)}))^T r_{(0)} &= 0 \\
(b - Ax_{(0)})^T r_{(0)} - \alpha (Ar_{(0)})^T r_{(0)} &= 0 \\
(b - Ax_{(0)})^T r_{(0)} &= \alpha (Ar_{(0)})^T r_{(0)} \\
r_{(0)}^T r_{(0)} &= \alpha r_{(0)}^T (Ar_{(0)}) \\
\alpha &= \frac{r_{(0)}^T r_{(0)}}{r_{(0)}^T A r_{(0)}}.
\end{aligned}
$$

$$
\alpha_{(i)} = \frac{r_{(i)}^T r_{(i)}}{r_{(i)}^T A r_{(i)}},
$$

$$
x_{(i+1)} = x_{(i)} + \alpha_{(i)} r_{(i)}.
$$

$$
r_{(i+1)} = r_{(i)} - \alpha_{(i)} A r_{(i)}.
$$

Taking fewer steps



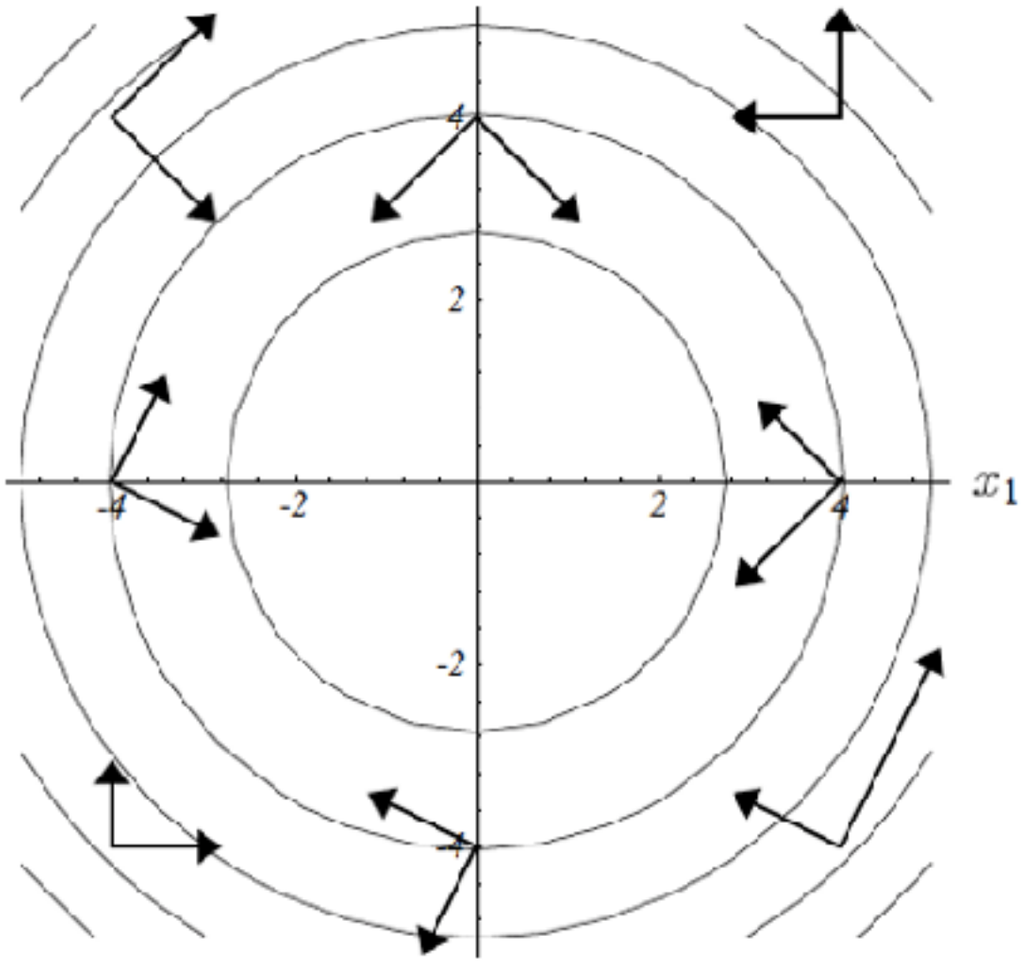
orthogonal *search directions* $d_{(0)}, d_{(1)}, \ldots, d_{(n-1)}$

$$x_{(i+1)} = x_{(i)} + \alpha_{(i)} d_{(i)}$$

$$\begin{aligned} d_{(i)}^T e_{(i+1)} &= 0 \\ d_{(i)}^T (e_{(i)} + \alpha_{(i)} d_{(i)}) &= 0 \\ \alpha_{(i)} &= -\frac{d_{(i)}^T e_{(i)}}{d_{(i)}^T d_{(i)}} \end{aligned}$$

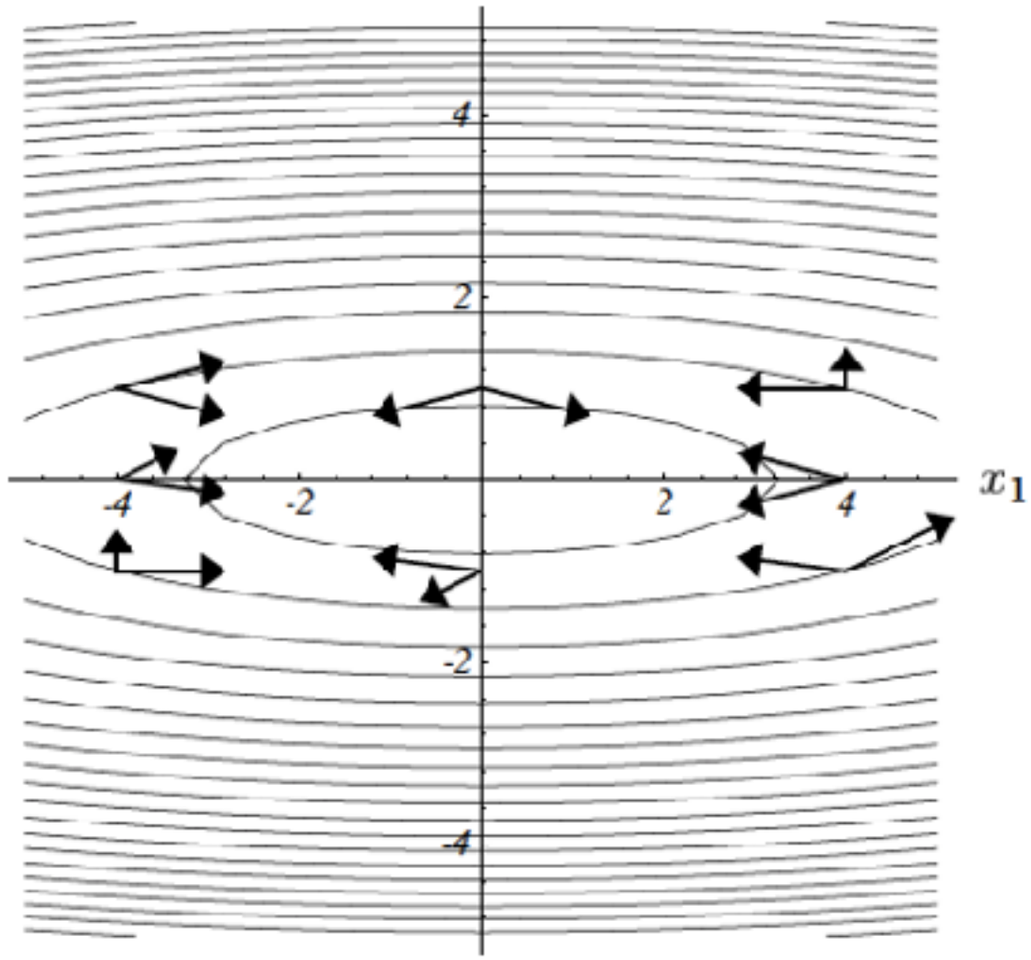
if we knew $e_{(i)}$, the problem would already be solved

Conjugate direction



orthogonal

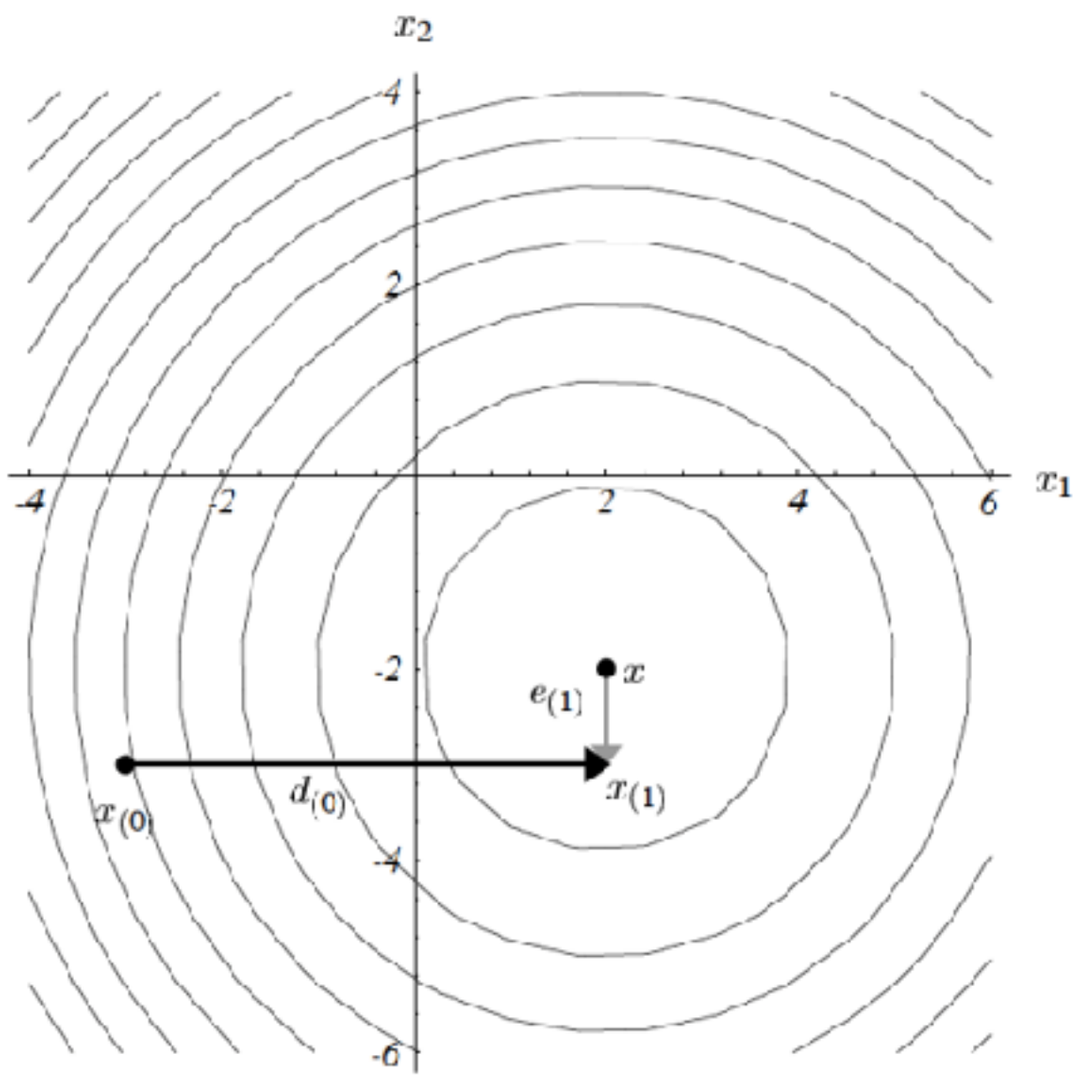
$$d_{(i)}^T d_{(i)} = 0$$



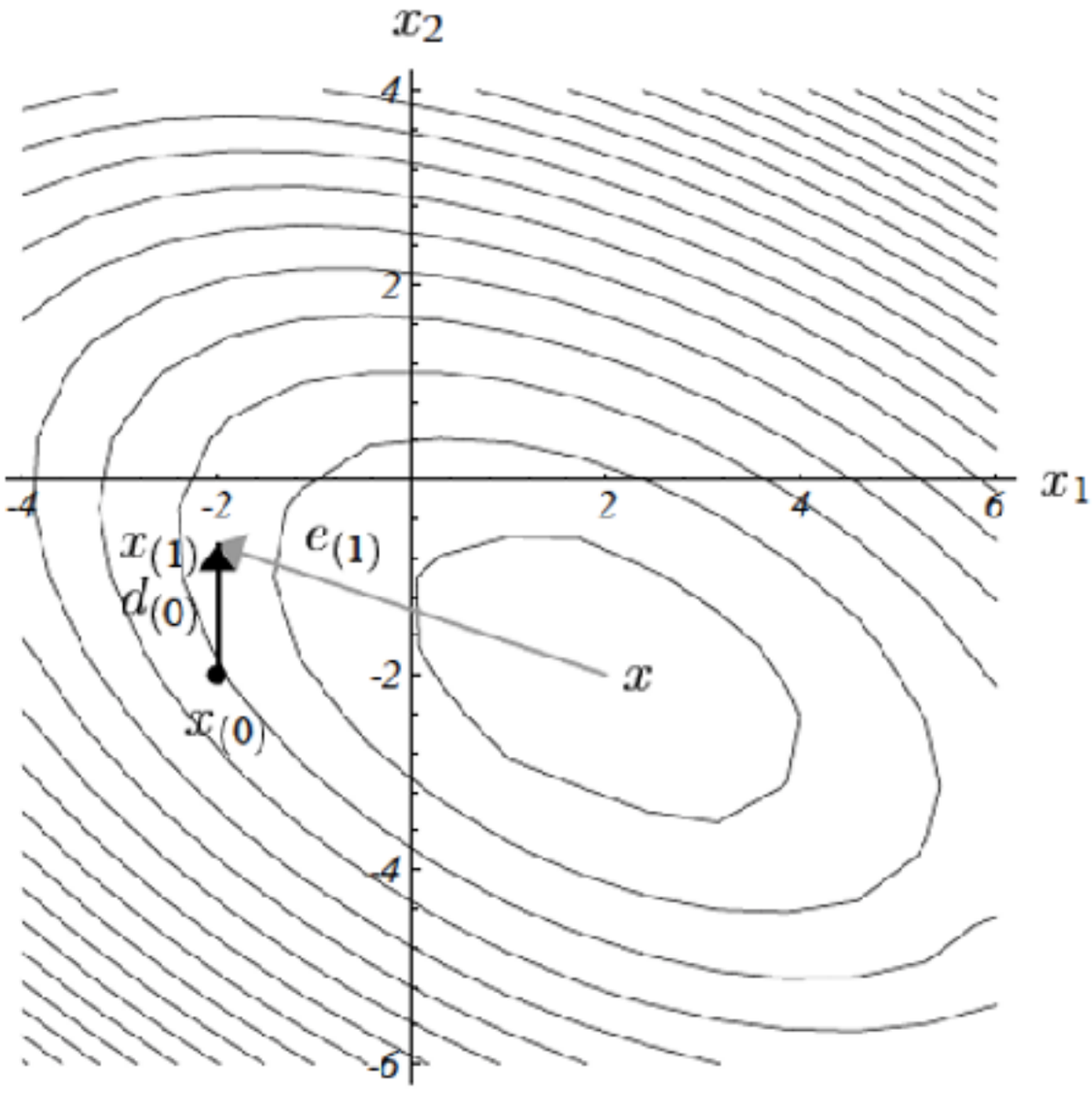
A-orthogonal $=$ *conjugate*

$$d_{(i)}^T A d_{(j)} = 0$$

Conjugate direction



$$\alpha_{(i)} = -\frac{d_{(i)}^T e_{(i)}}{d_{(i)}^T d_{(i)}}$$

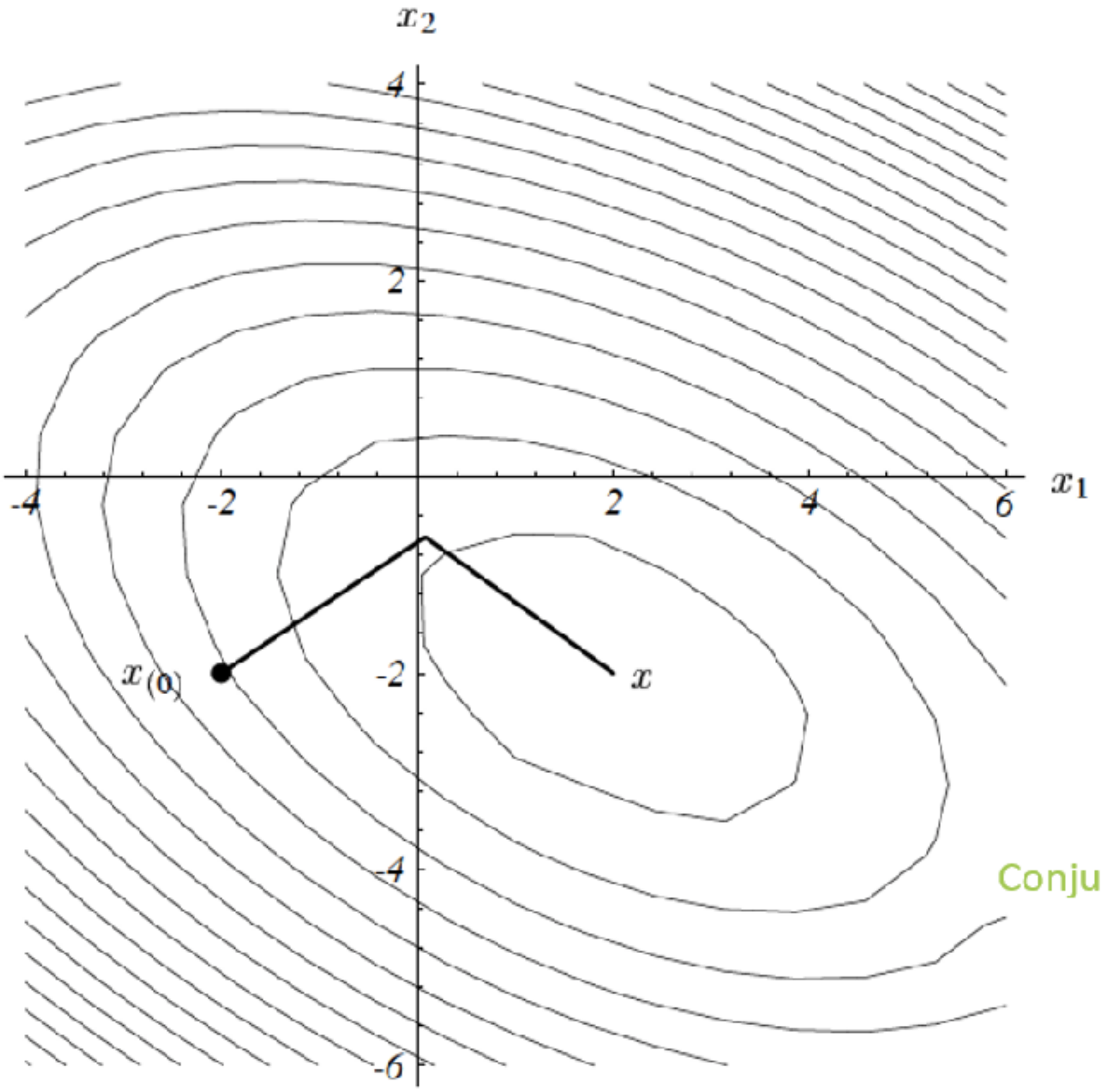


$$\alpha_{(i)} = -\frac{d_{(i)}^T A e_{(i)}}{d_{(i)}^T A d_{(i)}}$$

$$= \frac{d_{(i)}^T r_{(i)}}{d_{(i)}^T A d_{(i)}}.$$

~~if we knew $e_{(i)}$, the problem would already be solved~~

Conjugate gradient



$$d_{(0)} = r_{(0)} = b - Ax_{(0)}$$

$$\alpha_{(i)} = \frac{r_{(i)}^T r_{(i)}}{d_{(i)}^T A d_{(i)}}$$

$$x_{(i+1)} = x_{(i)} + \alpha_{(i)} d_{(i)},$$

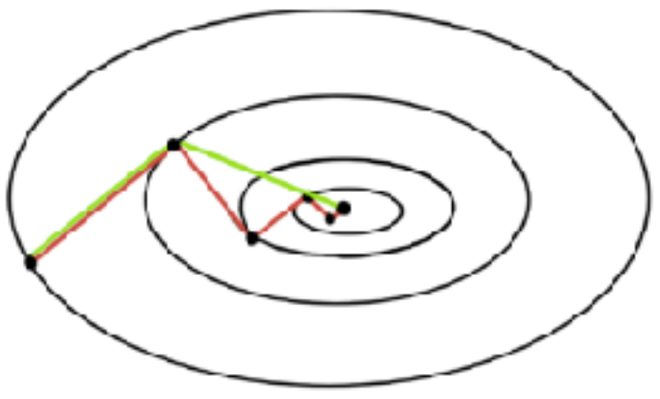
$$r_{(i+1)} = r_{(i)} - \alpha_{(i)} A d_{(i)},$$

$$\beta_{(i+1)} = \frac{r_{(i+1)}^T r_{(i+1)}}{r_{(i)}^T r_{(i)}},$$

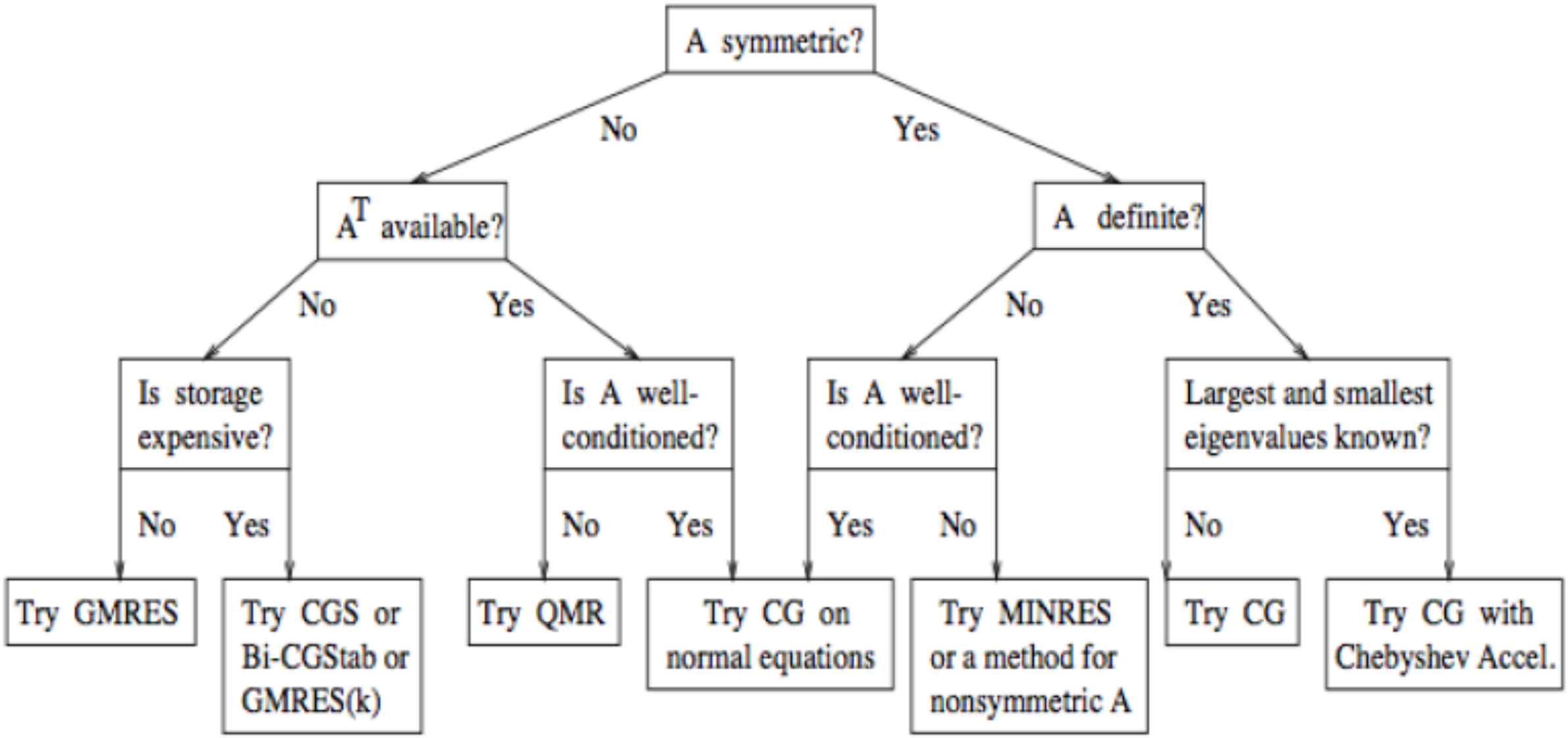
$$d_{(i+1)} = r_{(i+1)} + \beta_{(i+1)} d_{(i)}$$

Steepest decent

Conjugate gradient



Choosing a Krylov method



source: J. Demmel

Preconditioning