Iterative Solution of Sparse Matrices

Prateek Sharma (prateek@physics.iisc.ernet.in)
Office: D2-08

read “Painless Conjugate-Gradient” article for details

Iterative Methods

$$Ax = b$$

huge/important topic of iterative solution:
very useful for sparse, well-behaved, physical matrices.

e.g., *Jacobi relaxation*; A=D(diagonal matrix)+E(0 diagonal elements)

$$\begin{aligned} Dx &= -Ex + b \\ x &= -D^{-1}Ex + D^{-1}b \\ x &= Bx + z, \qquad \text{where} \quad B = -D^{-1}E, \qquad z = D^{-1}b. \end{aligned}$$

matrix-vector product is fast to evaluate for sparse matrices

iterative method: $x_{(i+1)} = Bx_{(i)} + z.$

$error\ e_{(i)} = x_{(i)} - x$ $\qquad e_{(i+1)} = Be_{(i)}$

converges if largest eigenvalue
(*spectral radius* $\rho_B<1$)

An Example

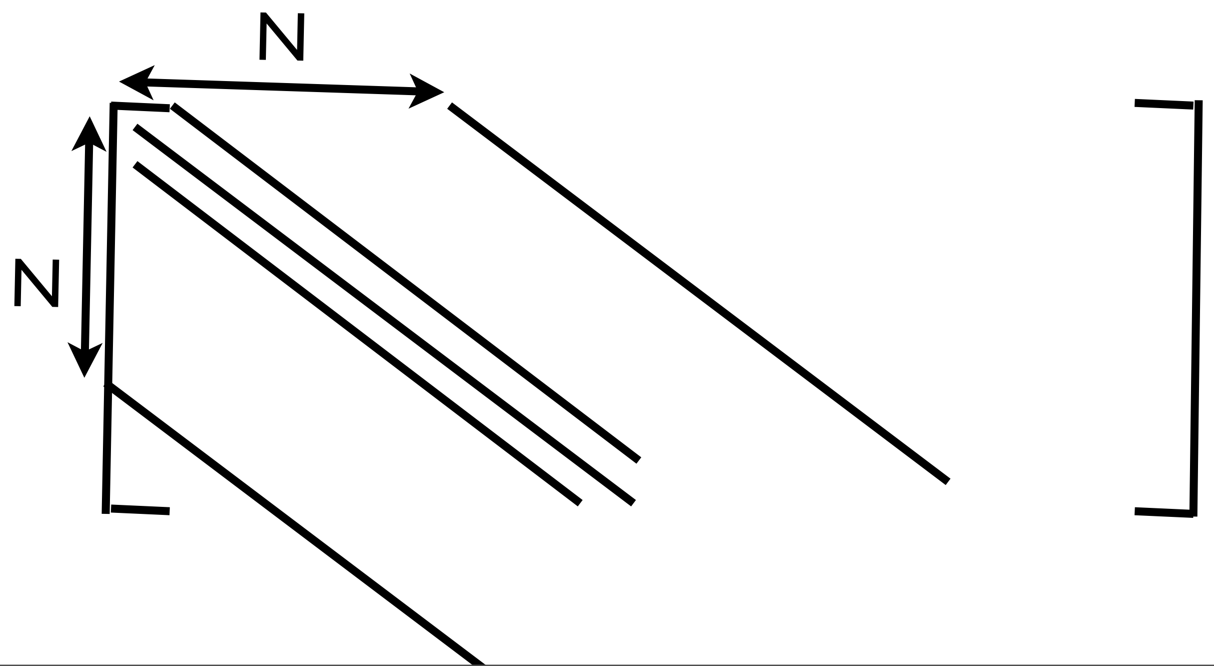
$$\nabla^2\Phi = 4\pi G\rho$$

Poisson equation

$$\begin{bmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & & \dots & & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \end{bmatrix} \Phi/h^2 = f$$

can be solved exactly in O(N) via tridiagonal

in 2D:



several bands separated by N-1 zeros
no fast method to solve it!

Jacobi is as good as in 1-D

Steepest Descent

N linear equations => fn. minimization in N-dimensional space

positive definite $x^T A x > 0.$ for every x; positive eigenvalues

class of general methods: step some in *search directions* till convergence
for symmetric, positive definite A (a lot of physics eqs. are of this class)

-only reference A via multiplication to a vector (don't need A explicitly); Av fast for sparse matrices

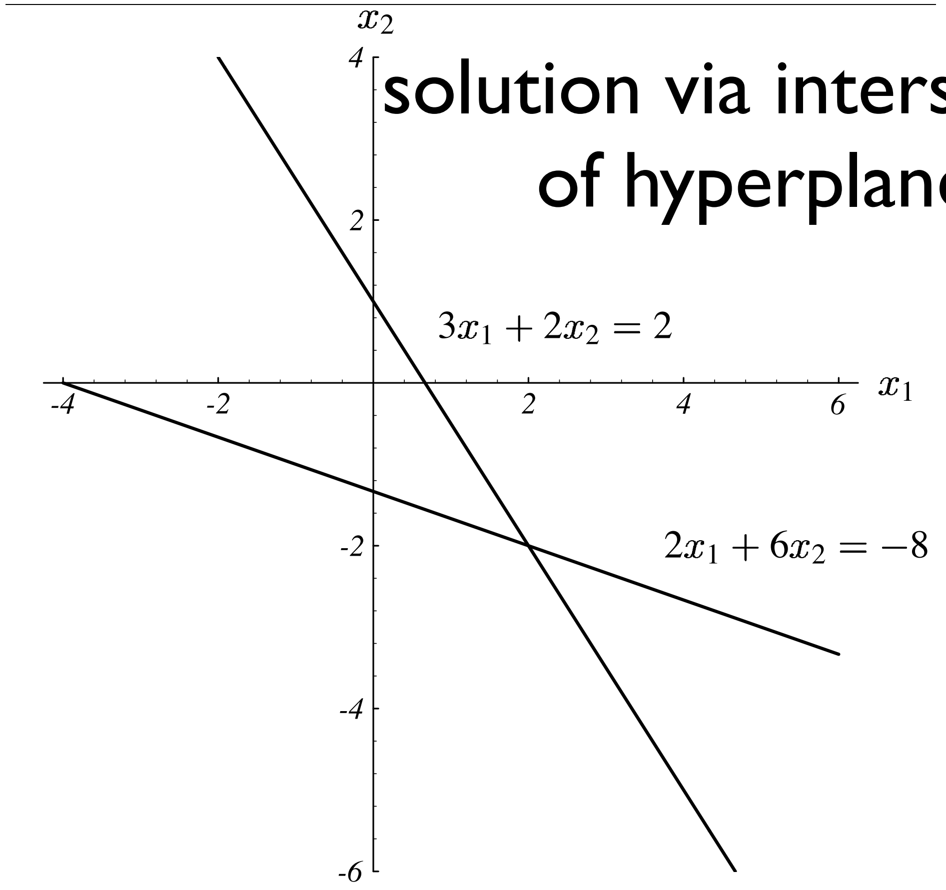
quadratic form:
minimized at root x

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

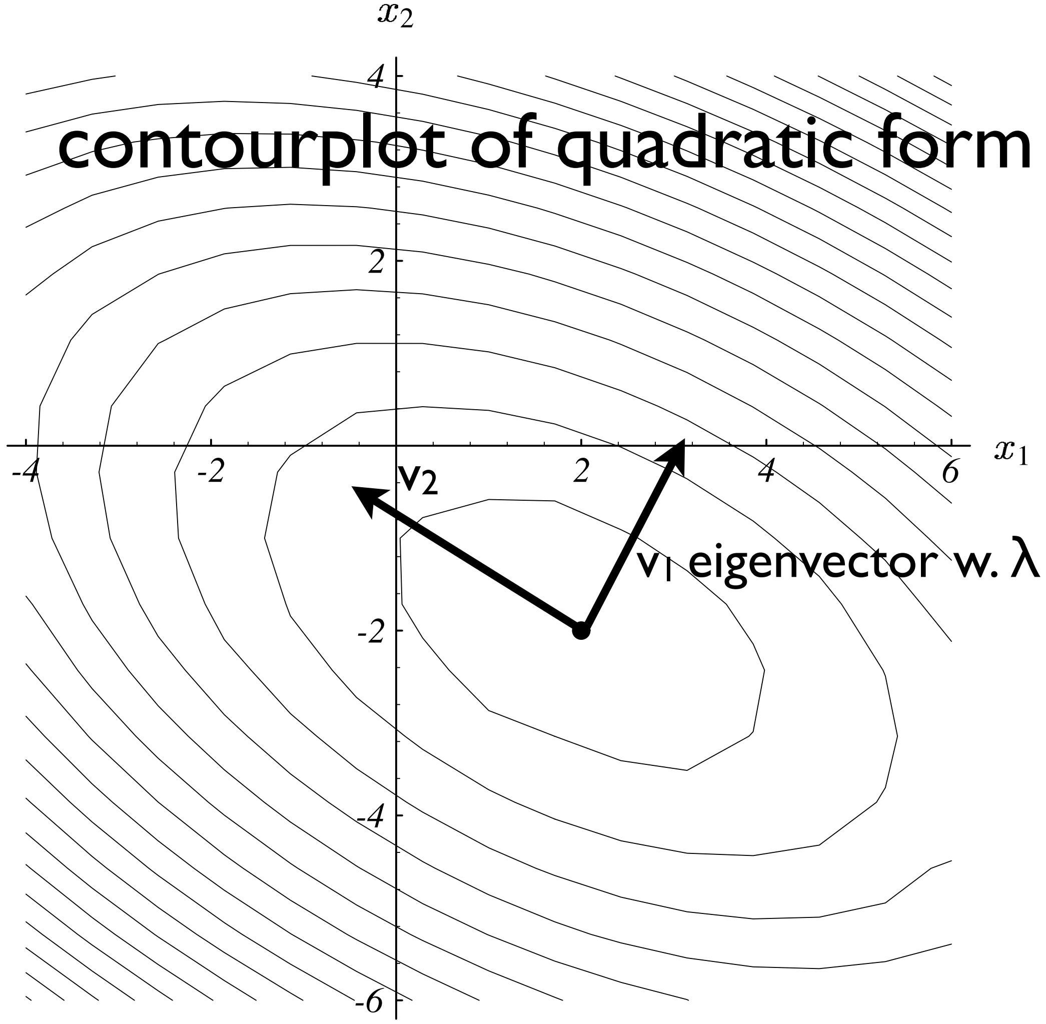
$f(x)$ is minimized by the solution to $Ax = b$.

$$A = \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix}, \qquad b = \begin{bmatrix} 2 \\ -8 \end{bmatrix}, \qquad c = 0.$$

solution via intersection of hyperplanes

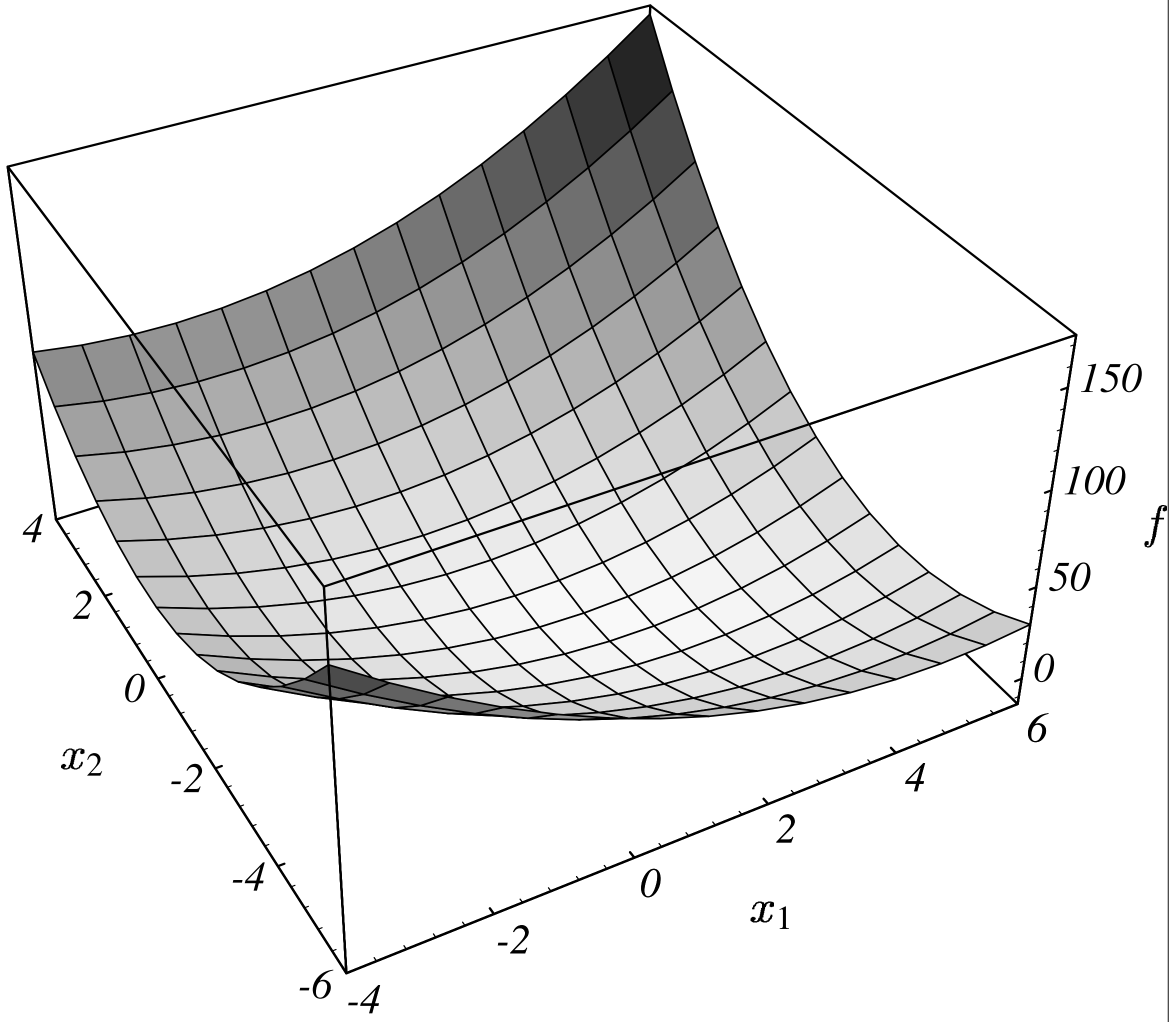


contourplot of quadratic form



v_2

v_1 eigenvector w. λ_1 , larger e.v.



surface plot of quadratic form

Properties of QF

$$f'(x) = \begin{bmatrix} \frac{\partial}{\partial x_1} f(x) \\ \frac{\partial}{\partial x_2} f(x) \\ \vdots \\ \frac{\partial}{\partial x_n} f(x) \end{bmatrix}$$

$$f'(x) = \frac{1}{2} A^T x + \frac{1}{2} A x - b.$$

$f'(x) = Ax - b.$ A is symmetric

f’ is along the direction of steepest ascent of f(x)

$f(p) = f(x) + \frac{1}{2}(p - x)^T A (p - x)$ => x (root) is minimum of f

Definitions

$$\mathit{error}\ e_{(i)} = x_{(i)} - x$$ unknown

$$\mathit{residual}\ r_{(i)} = b - Ax_{(i)}$$ known; projection onto A

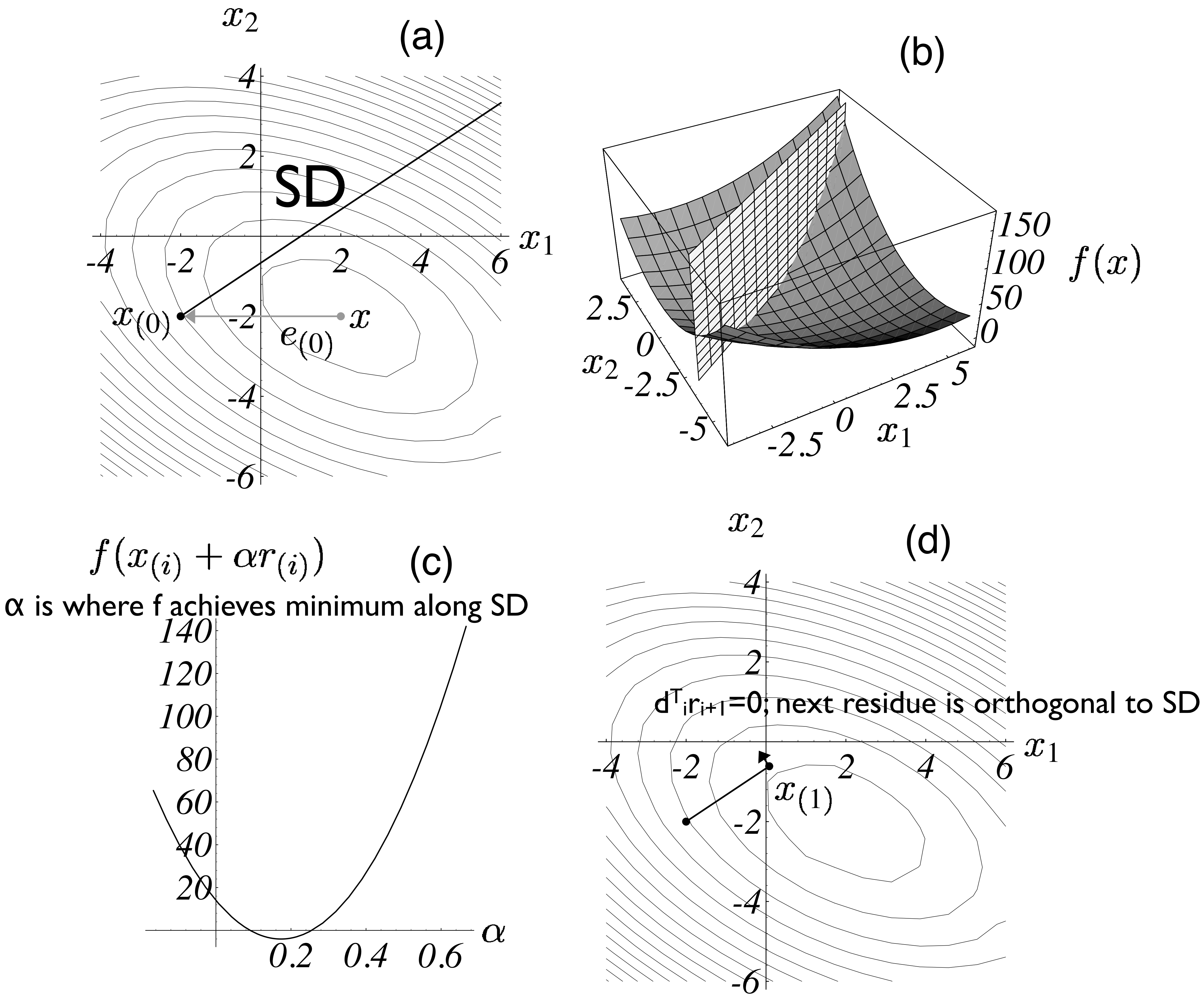
$$r_{(i)} = -Ae_{(i)} \qquad r_{(i)} = -f'(x_{(i)})$$

$$\mathit{line\ search} \qquad x_{(1)} = x_{(0)} + \alpha r_{(0)}$$ search dirn. $d_0 = r_0$

$$\frac{d}{d\alpha} f(x_{(1)}) = f'(x_{(1)})^T \frac{d}{d\alpha} x_{(1)} = f'(x_{(1)})^T r_{(0)}$$

for general SD

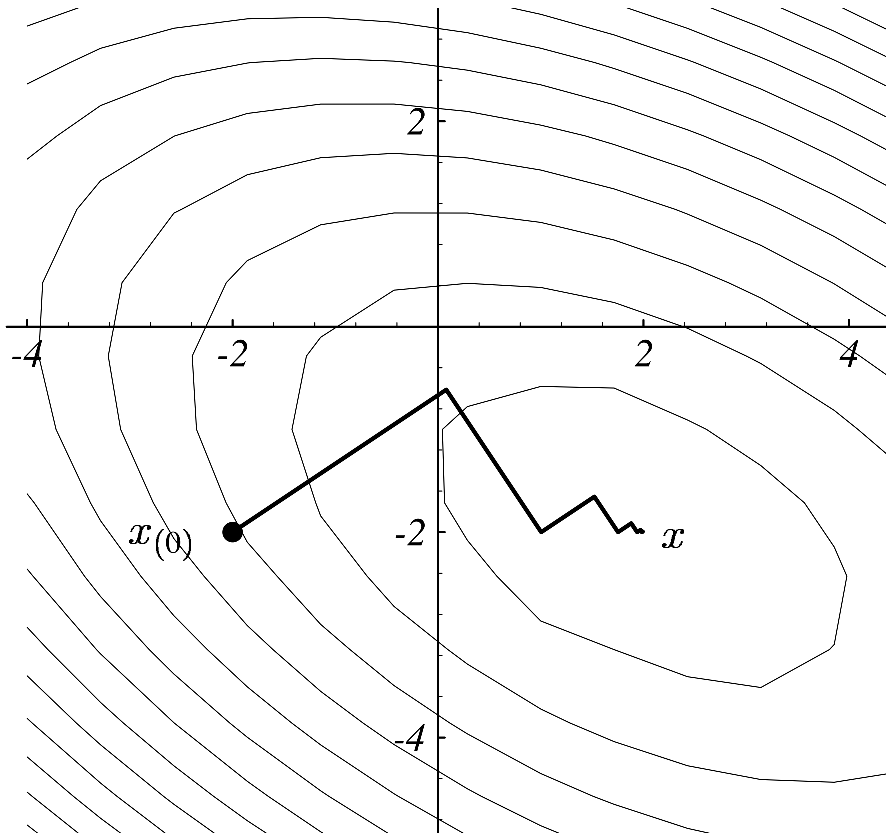
$$\begin{aligned} r_{(1)}^T r_{(0)} &= 0 \\ (b - Ax_{(1)})^T r_{(0)} &= 0 \end{aligned} \qquad \alpha = \frac{r_{(0)}^T r_{(0)}}{r_{(0)}^T A r_{(0)}} = \frac{d_{(i)}^T r_{(i)}}{d_{(i)}^T A d_{(i)}}.$$



SD

α is where f achieves minimum along SD

$d^T_i r_{i+1}=0$; next residue is orthogonal to SD



method of Steepest Descent is:

$$
\begin{aligned}
r_{(i)} &= b - Ax_{(i)}, \\
\alpha_{(i)} &= \frac{r_{(i)}^T r_{(i)}}{r_{(i)}^T A r_{(i)}}, \\
x_{(i+1)} &= x_{(i)} + \alpha_{(i)} r_{(i)}.
\end{aligned}
$$

error expanded as LC of independent eigenvectors

$$e_{(i)} = \sum_{j=1}^{n} \xi_j v_j,$$

$$r_{(i)} \;=\; -Ae_{(i)} = -\sum_j \xi_j \lambda_j v_j,$$

$$
\begin{aligned}
\|r_{(i)}\|^2 = r_{(i)}^T r_{(i)} &= \sum_j \xi_j^2 \lambda_j^2, \\
r_{(i)}^T A r_{(i)} &= \sum_j \xi_j^2 \lambda_j^3.
\end{aligned}
$$

$$
\begin{aligned}
e_{(i+1)} &= e_{(i)} + \frac{r_{(i)}^T r_{(i)}}{r_{(i)}^T A r_{(i)}} r_{(i)} \\
&= e_{(i)} + \frac{\sum_j \xi_j^2 \lambda_j^2}{\sum_j \xi_j^2 \lambda_j^3} r_{(i)}
\end{aligned}
$$

convergence of SD

$$\begin{aligned} \|e_{(i+1)}\|_A^2 &= e_{(i+1)}^T A e_{(i+1)} \\ &= \|e_{(i)}\|_A^2 \omega^2, \end{aligned} \qquad \omega^2 = 1 - \frac{(\sum_j \xi_j^2 \lambda_j^2)^2}{(\sum_j \xi_j^2 \lambda_j^3)(\sum_j \xi_j^2 \lambda_j)}$$

$$\begin{aligned} \omega^2 &= 1 - \frac{(\xi_1^2\lambda_1^2 + \xi_2^2\lambda_2^2)^2}{(\xi_1^2\lambda_1 + \xi_2^2\lambda_2)(\xi_1^2\lambda_1^3 + \xi_2^2\lambda_2^3)} \\ &= 1 - \frac{(\kappa^2 + \mu^2)^2}{(\kappa + \mu^2)(\kappa^3 + \mu^2)} \end{aligned}$$

amplification factor max when μ=κ

$$\omega \leq \frac{\kappa - 1}{\kappa + 1}.$$

condition number

determines rate of conv.

$$\kappa = \lambda_{max}/\lambda_{min},$$

$$\begin{aligned} \frac{f(x_{(i)}) - f(x)}{f(x_{(0)}) - f(x)} &= \frac{\frac{1}{2}e_{(i)}^T A e_{(i)}}{\frac{1}{2}e_{(0)}^T A e_{(0)}} \\ &\leq \left(\frac{\kappa - 1}{\kappa + 1}\right)^{2i}. \end{aligned}$$

Conjugate Directions

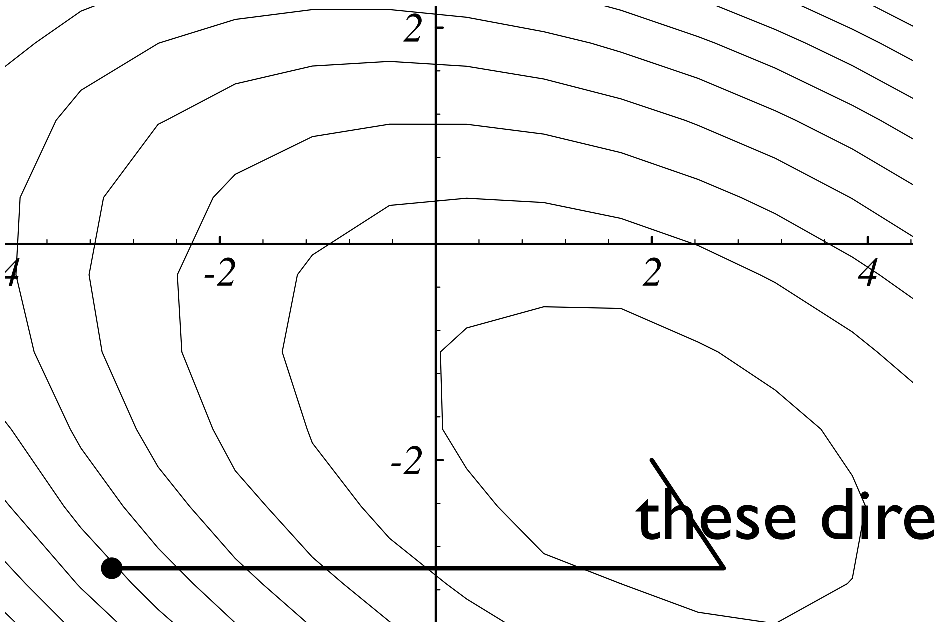
Gram-Schmidt Conjugation

construct A-orthogonal vectors (d_i) from a set of LI vectors (u_i), for i=0,..,n-1

$$d_{(i)} = u_i + \sum_{k=0}^{i-1} \beta_{ik} d_{(k)}, \quad \beta_{ij} \quad = \quad -\frac{u_i^T A d_{(j)}}{d_{(j)}^T A d_{(j)}}$$

s.t., $d^T_i d_j=0$ for i≠j

$\mathcal{O}(n^3)$



with A-orthogonal SDs convergence is guaranteed in n steps, unlike SD

these directions are orthogonal if eigenvector directions are normalized by eigenvalues of A

Conjugate Gradients

CG is method of conjugate directions where LI vectors to be conjugated to form SDs are $\{r_0, r_1, ..., r_{n-1}\}$

since error after n steps is zero!

$$r_{(i+1)} = r_{(i)} - \alpha_{(i)} A d_{(i)} \qquad 0 = \sum_{j=i}^{n-1} \alpha_{(i)} d_{(i)} + e_{(j)}$$

$$r_{(i)}^T r_{(j)} = 0, \qquad i \neq j.$$

since d_is are conjugate (A-orthogonal)

$$\mathcal{D}_i = \text{span}\{d_{(0)}, d_{(1)}, \ldots, d_{(i-1)}\}$$

$\mathcal{D}_{i+1}$ is formed from the union of the previous subspace $\mathcal{D}_i$ and the subspace $A\mathcal{D}_i$

Krylov subspace

$$\mathcal{D}_i = \text{span}\{r_{(0)}, Ar_{(0)}, A^2 r_{(0)}, \ldots, A^{i-1} r_{(0)}\}$$

CG method

only r_i, r_{i-1} needed to construct d_i; constructing conjugate basis cheap!

$$d_{(i)} = u_i + \sum_{k=0}^{i-1} \beta_{ik} d_{(k)},$$

$$\begin{aligned} r_{(i)}^T r_{(j+1)} &= r_{(i)}^T r_{(j)} - \alpha_{(j)} r_{(i)}^T A d_{(j)} \\ \alpha_{(j)} r_{(i)}^T A d_{(j)} &= r_{(i)}^T r_{(j)} - r_{(i)}^T r_{(j+1)} \\ r_{(i)}^T A d_{(j)} &= \begin{cases} \frac{1}{\alpha_{(i)}} r_{(i)}^T r_{(i)}, & i = j, \\ -\frac{1}{\alpha_{(i-1)}} r_{(i)}^T r_{(i)}, & i = j+1, \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

$$\therefore \beta_{ij} = \begin{cases} \frac{1}{\alpha_{(i-1)}} \frac{r_{(i)}^T r_{(i)}}{d_{(i-1)}^T A d_{(i-1)}}, & i = j+1, \\ 0, & i > j+1. \end{cases}$$

$$\beta_{(i)} = \beta_{i,i-1}$$

$$\begin{aligned} \beta_{(i)} &= \frac{r_{(i)}^T r_{(i)}}{d_{(i-1)}^T r_{(i-1)}} \\ &= \frac{r_{(i)}^T r_{(i)}}{r_{(i-1)}^T r_{(i-1)}} \end{aligned}$$

$$\begin{aligned} d_{(i)}^T r_{(j)} &= u_i^T r_{(j)} + \sum_{k=0}^{i-1} \beta_{ik} d_{(k)}^T r_{(j)} \\ 0 &= u_i^T r_{(j)}, \qquad i < j \end{aligned}$$

since $d_{(i)}^T r_{(i)} = u_i^T r_{(i)}$

CG algorithm

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

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

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

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

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

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

condn. no.

$$\|e_{(i)}\|_A \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^i \|e_{(0)}\|_A$$

faster conv. than SD

dominating operations during an iteration of either Steepest Descent or CG are matrix-vector products

matrix-vector multiplication requires $\mathcal{O}(m)$ operations, where m is the number of non-zero entries

SD

$$i \leq \left\lceil \frac{1}{2} \kappa \ln \left(\frac{1}{\epsilon} \right) \right\rceil$$

CG

$$i \leq \left\lceil \frac{1}{2} \sqrt{\kappa} \ln \left(\frac{2}{\epsilon} \right) \right\rceil$$

I conclude that Steepest Descent has a time complexity of $\mathcal{O}(m\kappa)$, whereas CG has a time complexity of $\mathcal{O}(m\sqrt{\kappa})$. Both algorithms have a space complexity of $\mathcal{O}(m)$.

$\kappa \in \mathcal{O}(n^{2/d})$ second-order elliptic boundary value problems m~n^{d-1}, d:dim.