Linear Least Square

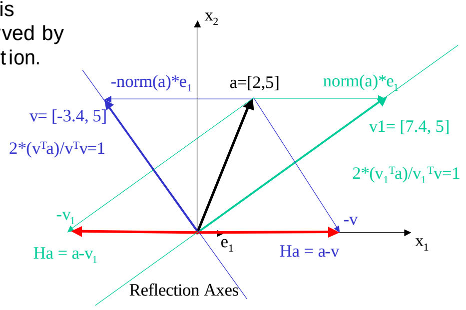
- Often we have more equations than unknowns, because, for example, some experiments have been repeated several time,
- We obtain different results because of different input data.
- These results are arranged by more equations m than unknowns n. The transformation A has dimensions mxn. Columns of A span n-dimensional vector space.
- Resulting system $Ax \approx b$ is solved in the best way if the residual $r=b-Ax$ is minimal, so the best fitting x to the existing data b is obtained.

Linear Transformations

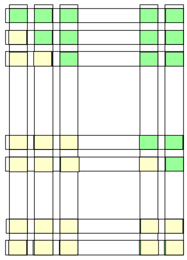
- A linear transformation A in general changes the length and the direction of a vector x.
- Some special transformations are often needed that preserve vector norms - orthogonal transformations.
- A solution is the best possible, if the residual is minimal, that is, if it is orthogonal (perpendicular) to the column space of A.
- So we have to solve least squares problem by a smaller square system but triangular matrix has to be obtained by an orthogonal transformation that will preserve the solution.

Housholder Transformation

Norm is preserved by reflection.



Housholder QR Factorization



```
for j=1:n % for each column j
  n=norm(A(j:m,j)) % column norm
  v=A(j:m,j)-n*e_j % vector v
  for i=j:n %update all unfactorized
    for k=j:m % column entries
      A(k,i)=A(k,i)-(2*(v'*A(k,i))/(v'*v))*v;
    end
  end
end
```

We must update b also, transforming the system A*x=b in $R*x=Q^T*b(1:n)$

Complexity: **$O(n^2m-n^3/3)$**

Givens Rotation

- Rotation,
- Norm preserved.

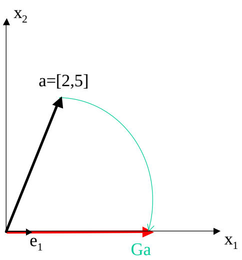
norm(a)=sqrt($a_1^2 + a_2^2$)=5.39

c= a_1 /norm(a)=0.37

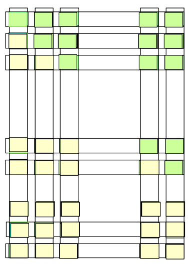
s= a_2 /norm(a)=0.93

G= [c s; -s c]=[.37 .93; -.93 .37]

Ga=[5.39, 0]



Givens QR Factorization



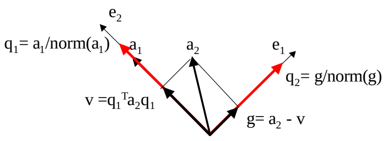
```
for j=1:n % for each column j
  for k=m:-1:j+1 % from bottom
    c=A(k-1,j)/sqrt(A(k,j)); % c
    s=A(k,j)/sqrt(A(k,j)); % s
    G(k-1,k-1)=c; Gi(k,k)=c;
    G(k,k-1)=-s; Gi(k-1,k)=s;
    A=G*A; %update matrix A
  end
end
```

We must update b also, transforming the system A*x=b in $R*x=Q^T*b(1:n)$

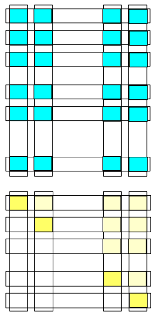
Complexity: **$O(n^2m-n^3/2)$** (50% more than Housholder)

Grahm-Schmidt Orthogonalization

- Orthogonalization,
- Norm preserved.



Modified Gram-Schmidt QR Factorization



```
R=zeros(m,n) % place for R
for k=1:n % for each column k of A
  R(k,k)=norm(A(:,k)); % column norm
  A(:,k)= A(:,k)/ R(k,k) % normalize
  for j=k+1:n % for all unfactor.colu.
    R(k,j)=A(:,k)*A(:,j) % orthogonalize
    A(:,j)=A(:,j)-R(k,j)*A(:,k) % update
  end
end
```

Extra space is needed for R!

We must update b also, transforming the system $A*x=b$ in $R*x=Q^T*b$

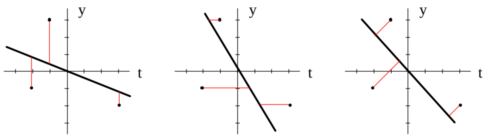
Complexity: **$O(n^2m-n^3)$**

Total Least Squares

f(t,x)=xt

t	-2	-1	3
y	-1	3	-2

Ordinary Least Square   Total Least Square



[t]*x = [y]   [y]*x = [t]   [t,y]=UΣV' $x=-v_{1,2}/v_{2,2}$

vertical distances   horizontal distances   perpendicular distances