CS 357: Numerical Methods

Lecture 11: QR Decomposition

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Why is orthogonality useful?

- Matrices with orthonormal columns can do special things
- **Qv** preserves the 2-norm of **v**
- Important in Least Squares problems

Orthogonal Transformations Preserve the 2-Norm

- What is true about the columns of an orthonormal matrix Q?
- What is QQ^T ?

Orthogonal Transformations Preserve the 2-Norm

We can show that $\|Qv\|_2^2 = \|v\|_2^2$

Orthogonal Transformations Preserve the 2-Norm

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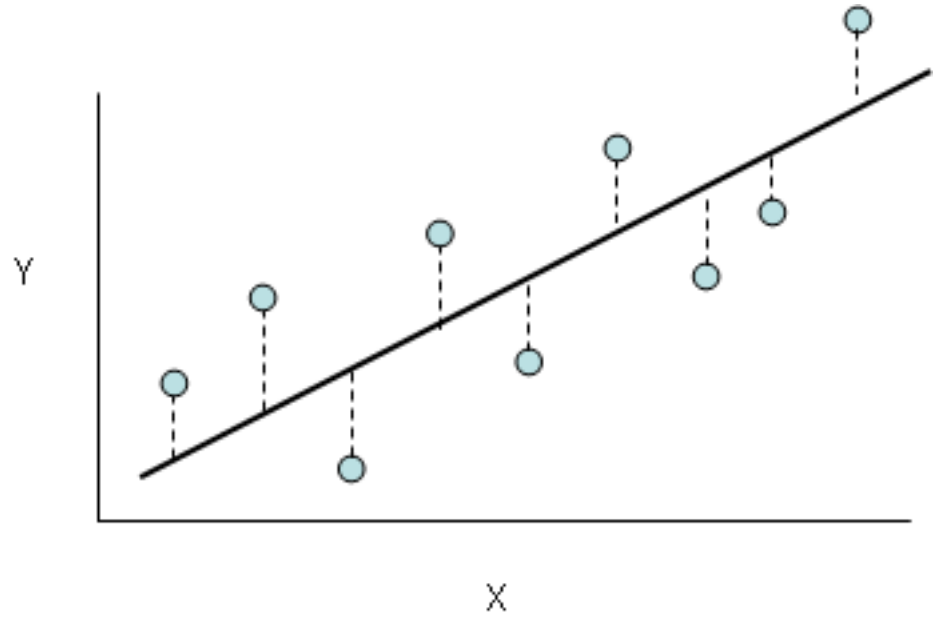
Orthogonal Transformations Preserve the 2-Norm

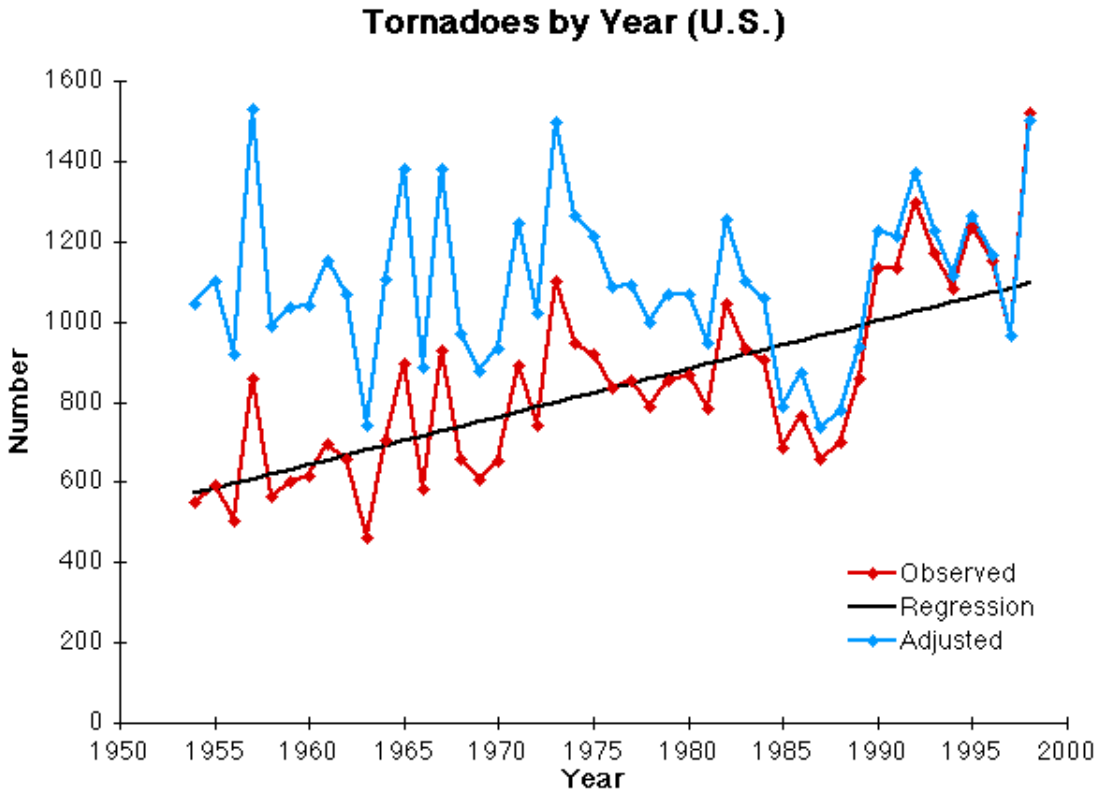
- What does this mean in terms of amplifying error?

Least Squares Problems

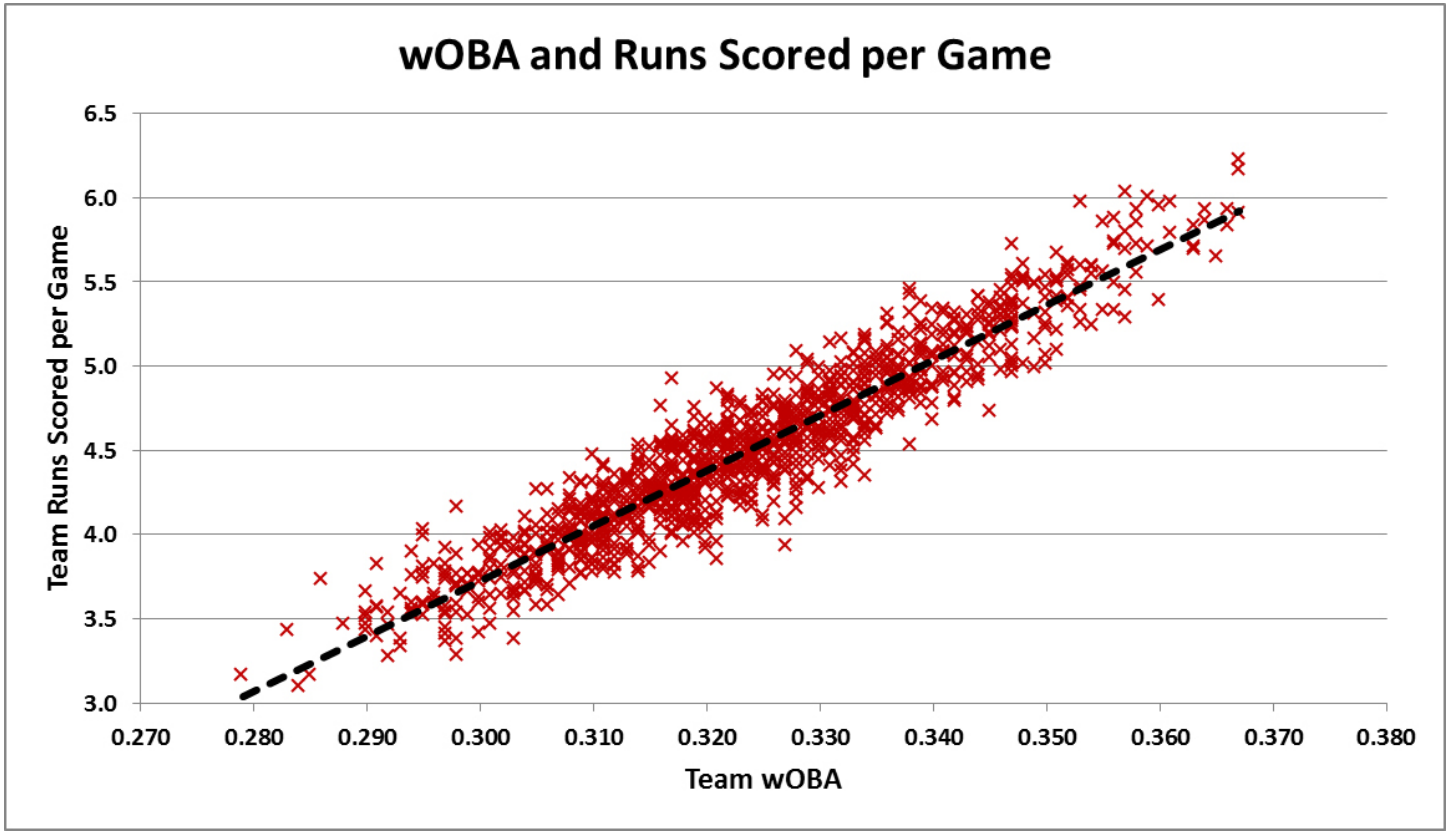
- Lots of interesting problems lack an exact solution….
- Fit a line to a set of points….



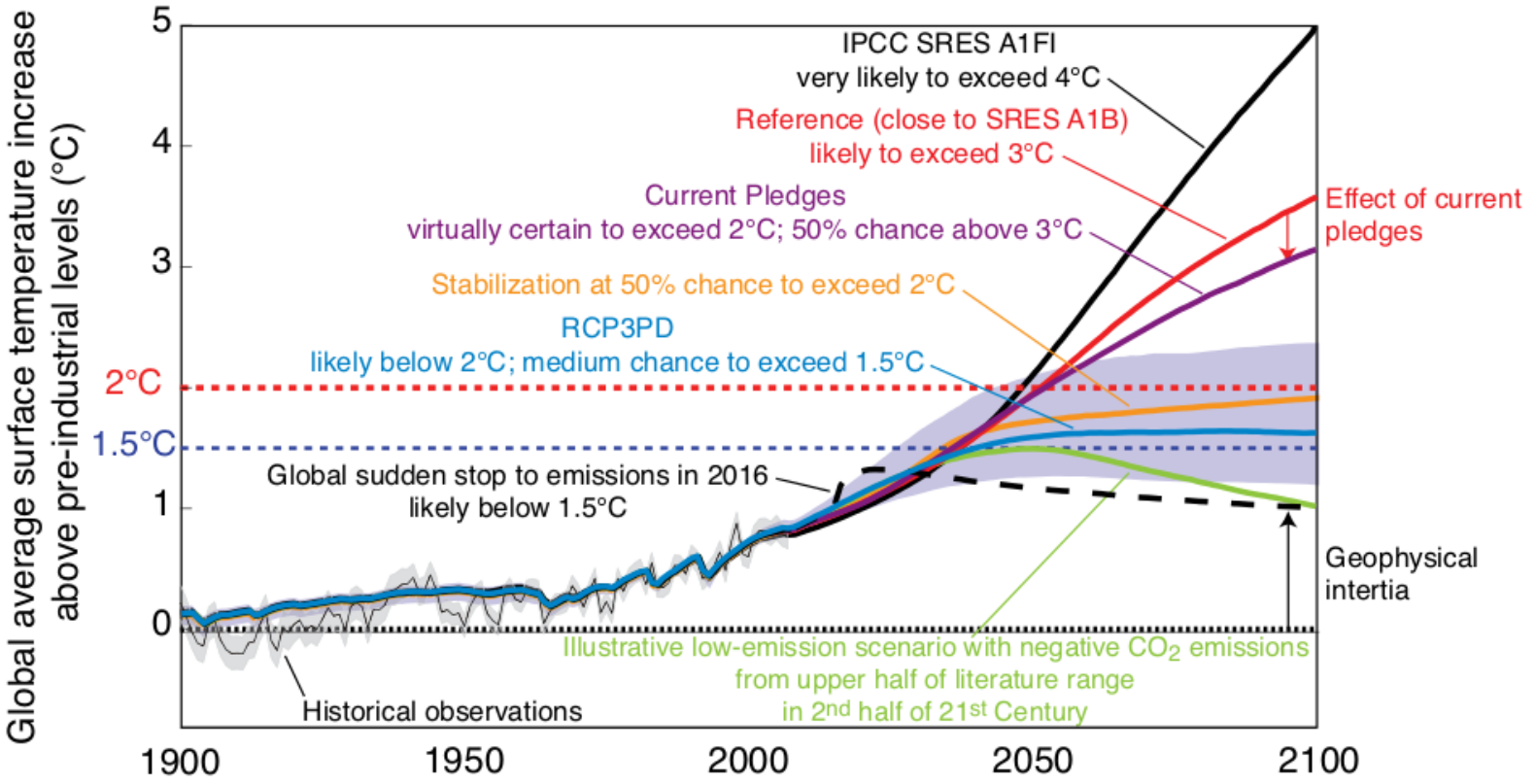
Least Squares Applications



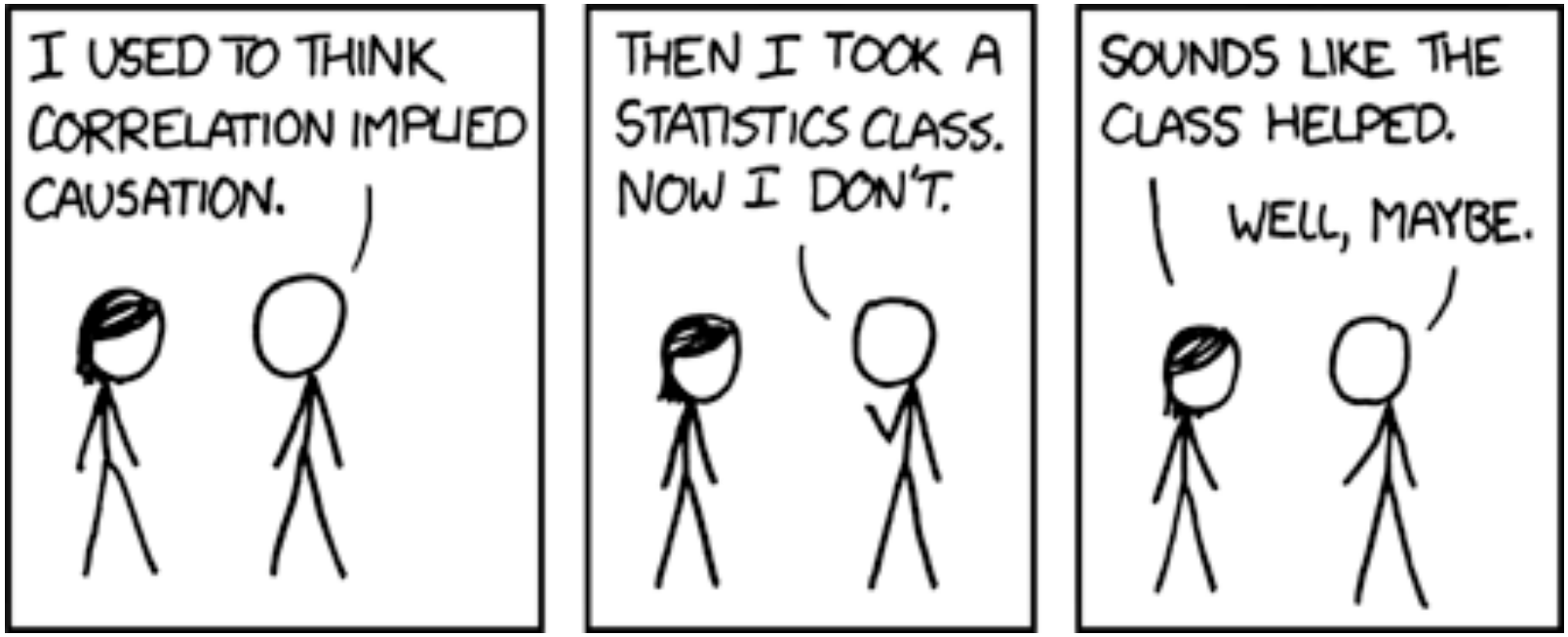
Least Squares Applications



Least Squares Applications



Beware: correlation and causation



Preview: Least Squares as Linear Algebra

Let's fit a line to series of data sampled over times t_0, t_1, t_2…,t_{m-1}

The line is given by $f(t) = x_1 t + x_0$

So…how does orthogonality relate to least squares?

- The closest fit to the observed data is an orthognonal projection into the column space of a matrix….
  - You'll understand later….

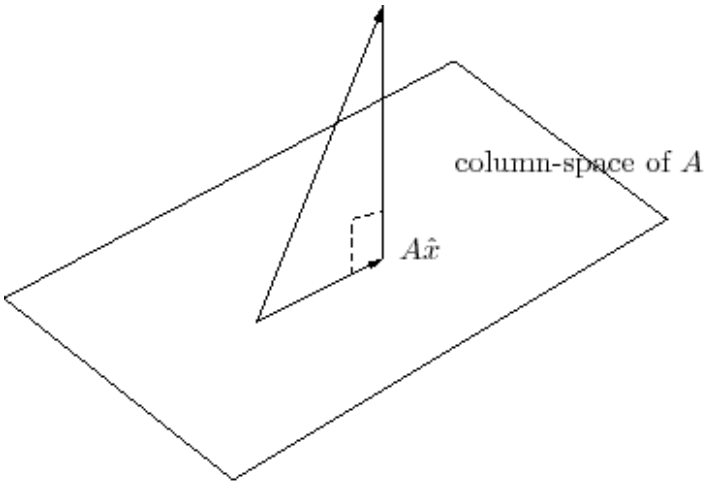


Figure J.1: Geometrical interpretation of orthogonal projection.

Recap: Orthonormal Basis

- A basis is orthonormal if each basis vector:
  - Has unit length
  - Is orthogonal to all other basis vectors.

- Example: (1,0) and (0,1) for 2D Euclidean space
- Can you give another 2D orthonormal basis?

Recap: Orthonormal Basis

For some given vector $\vec{x}$, how do I find coefficients with respect to an ONB?

$$\vec{x} = (x \cdot b_1)\,\vec{b}_1 + (x \cdot b_2)\,\vec{b}_2 + (x \cdot b_3)\,\vec{b}_3 + \cdots + (x \cdot b_n)\,\vec{b}_n$$

Much easier than finding coefficients by solving a linear system!

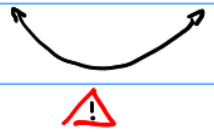
Also much cheaper: $O(n^2)$

Recap: Orthonormal Basis

Can we build a matrix that computes those coefficients for us?

$$Q = \begin{pmatrix} | & & | \\ \vec{b}_1 & \cdots & \vec{b}_n \\ | & & | \end{pmatrix} \rightsquigarrow Q^T \vec{x} = \begin{pmatrix} \vec{b}_1 \cdot \vec{x} \\ \vdots \\ \vec{b}_n \cdot \vec{x} \end{pmatrix}$$

A square matrix whose columns are orthonormal is called orthogonal.



Example

Orthogonal Projection

What if Q contains a few zero columns instead of orthonormal vectors?

$Q = \left[\begin{array}{ccc|c} | & & | & \\ \vec{b}_1 & \cdots & \vec{b}_k & 0 \\ | & & | & \end{array}\right]$

orthonormal columns

Define $P := QQ^T$

Compute $P\vec{x}$ for $\vec{x} = \alpha_1\vec{b}_1 + \cdots + \alpha_n\vec{b}_n$:

$$Q^T\vec{x} = \begin{pmatrix} \vec{x}\cdot\vec{b}_1 \\ \vdots \\ \vec{x}\cdot\vec{b}_k \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Orthogonal Projection

Define $P := QQ^T$

Compute $P\vec{x}$ for $\vec{x} = \alpha_1\vec{b}_1 + \cdots + \alpha_n\vec{b}_n$:

$$Q^T\vec{x} = \begin{pmatrix} \vec{x}\cdot\vec{b}_1 \\ \vdots \\ \vec{x}\cdot\vec{b}_k \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$Q(Q^T\vec{x}) = \underbrace{(\vec{x}\cdot\vec{b}_1)\vec{b}_1 + \cdots + (\vec{x}\cdot\vec{b}_k)\vec{b}_k}_{\text{x projected onto } \vec{b}_1 \cdots \vec{b}_k} + \underbrace{0\cdot\vec{b}_{k+1} + \cdots + 0\cdot\vec{b}_n}_{\vec{0}}$$

Example

Gram-Schmidt Orthogonalization

- Given linearly independent a1 and a2
- Find q1 and q2 that are orthonormal and span same space

Classical Gram-Schmidt

- We can orthogonalize any number of vectors…

```
for k in range(A.shape[1]):
    avec = A[:, k]
    q = avec
    for j in range(k):
        q = q - np.dot(avec, Q[:,j])*Q[:,j]

    Q[:, k] = q/la.norm(q)
```

Problems

- Rounding error can destroy orthogonality in the q_k vectors
- Also we need to store A, Q and R separately
  - problematic for large systems

Modified Gram-Schmidt

```
for k in range(A.shape[1]):
    q = A[:, k]
    for j in range(k):
        q = q - np.dot(q, Q[:,j])*Q[:,j]

    Q[:, k] = q/la.norm(q)
```