

## Unit III

### Curve-Fitting and Interpolation

## Curve-fitting and interpolation

- Curve fitting
  - linear least squares fitting problem
  - transformations to linearize nonlinear problems
  - three solution techniques:
    - normal equations
    - QR decomposition
    - SVD
- Interpolation
  - polynomial interpolation
  - piecewise polynomial interpolation
  - cubic splines

## Curve fitting

- finding an analytical function which approximates a set of data points
- statistics can quantify the relationship between the fit and errors in data points (e.g. from experiment)
- numerical methods is concerned with the calculation of the fitting curve itself

## **Linear** curve fitting

- consider a single variable problem initially
- start with  $m$  data points  $(x_i, y_i)$ ,  $i=1, \dots, m$
- choose  $n$  basis functions  $f_1(x), \dots, f_n(x)$
- define a fit function  $F(x) = c_1 f_1(x) + \dots + c_n f_n(x)$  as a **linear** combination of the basis functions
- the problem:
  - find the unknown coefficients  $c_1, \dots, c_n$  so that  $F(x_i) \approx y_i$
  - provide a means to quantify the fit

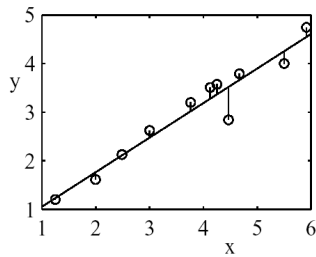
## Linear curve fitting

- in general  $m > n$ 
  - large number of data points
  - (much) smaller number of coefficients/basis functions
- so  $F(x_i) = y_i$  exactly is not possible to achieve
- fitting to a line uses two basis functions
  - $f_1(x) = x$
  - $f_2(x) = 1$
- the fitting function is  $F(x) = c_1 x + c_2$
- $m$  residuals are defined by
$$r_i = y_i - F(x_i) = y_i - (c_1 x_i + c_2)$$

## Least squares problem

- quality of fit can be measured by sum of squares of the residuals  $\rho = \sum r_i^2 = \sum [y_i - (c_1 x_i + c_2)]^2$ 
  - easy to calculate the fit coefficients
  - agrees with statistical expectations derived from data analysis
- minimizing  $\rho$  with respect to  $c_1$  and  $c_2$  provides the least-squares fit
  - data points  $x_i$  and  $y_i$  are known in expression for  $\rho$
  - only  $c_1$  and  $c_2$  are unknowns

## Least squares problem



## Geometry or algebra?

- to solve the least squares fitting problem we can ...
  - minimize the sum of squares (geometry) OR
  - solve the over-determined system (algebra)
- the equations you get are ...
  - mathematically the same, but
  - have significantly different numerical properties

## Geometric: Minimize the residual

- to minimize  $\rho = \rho(c_1, c_2)$  we must have the partial derivatives

$$\frac{\partial \rho}{\partial c_1} = \frac{\partial \rho}{\partial c_2} = 0$$

- differentiating gives (sums are  $i=1, \dots, m$ )

$$\frac{\partial \rho}{\partial c_1} = \sum \frac{\partial}{\partial c_1} [y_i - (c_1 x_i + c_2)]^2 = \sum -2x_i [y_i - (c_1 x_i + c_2)]$$

$$\frac{\partial \rho}{\partial c_2} = \sum \frac{\partial}{\partial c_2} [y_i - (c_1 x_i + c_2)]^2 = \sum -2[y_i - (c_1 x_i + c_2)]$$

## Minimize the residual

- to minimize we get

$$0 = \sum x_i y_i - c_1 \sum x_i^2 - c_2 \sum x_i$$

$$0 = \sum y_i - c_1 \sum x_i - c_2 m$$

- organizing in matrix form gives the *normal equations* for the least squares fit:

$$\begin{bmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & m \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} \sum x_i y_i \\ \sum y_i \end{bmatrix}$$

## Algebraic: Over-determined system

- formally write the equation of the line through all the points

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_m & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

- $Ac = y$  is an over-determined system
- it has an exact solution only if all the data points lie on a line, i.e.  $y$  is in the column space of  $A$

## Over-determined system

- a compromise solution can be found by minimizing the residual  $r = y - Ac$  (as defined in unit I)
- find the minimum of  $\rho = \|r\|_2^2$ 

$$= r^T r = (y - Ac)^T (y - Ac)$$

$$= y^T y - y^T Ac - c^T A^T y + c^T A^T Ac$$

$$= y^T y - 2y^T Ac + c^T A^T Ac \quad [\text{why?}]$$
- to minimize  $\rho$  requires that  $\partial \rho / \partial c = 0$ 
  - differentiation with respect to a vector  $c$
  - means a column vector of partial derivatives with respect to  $c_1, c_2$

## Digression: vector derivatives

- how to differentiate with respect to a vector?
- we need some properties of vector derivatives ...
  - $\partial(Ax)/\partial x = A^T$
  - $\partial(x^T A)/\partial x = A$
  - $\partial(x^T x)/\partial x = 2x$
  - $\partial(x^T Ax)/\partial x = Ax + A^T x$
- the notation convention for vector derivative  $\partial/\partial x$  is NOT standardized with respect to transposes:
  - disagrees with Jacobian matrix definition

## Over-determined system

- now evaluate:  $\partial \rho / \partial c = 0$
- $\partial \rho / \partial c = \partial / \partial c [y^T y - 2y^T A c + c^T A^T A c]$ 

$$= -2A^T y + [A^T A c + (A^T A)^T c]$$

$$= -2A^T y + 2A^T A c$$

$$= 0$$

## Normal equations again

- these give the normal equations again in a slightly different disguise:
 
$$A^T A c = A^T y$$
- these are the same equations as the normal equations derived previously from geometric reasoning
- to fit data to a line you can solve the normal equations for  $c$
- Matlab example: `linefit(x,y)`
  - fits data points by solving the normal equations using backslash

## Linearizing a nonlinear relationship

- a line can be fit to an apparently nonlinear relationship by using a transformation
- example: to fit  $y = c_1 \exp(c_2 x)$ 
  - take ln of both sides:  $\ln y = \ln c_1 + c_2 x$
  - put  $v = \ln y$ ,  $\alpha = \ln c_1$ ,  $\beta = c_2$  to linearize the problem
  - you get  $v = \alpha + \beta x$
  - fit the transformed data points:  $(x_i, v_i)$
- this procedure minimizes the residuals of the transformed data fitted to a line, NOT the residuals of the original data

## Generalizing to arbitrary basis functions

- $y = F(x) = c_1 f_1(x) + \dots + c_n f_n(x)$  is the general linear fit equation
- the basis functions  $f_j \dots$ 
  - are independent of the coefficients  $c_j$
  - may be individually nonlinear
- $F(x)$  itself is a linear combination of the  $f_j$
- as before we can write the general over-determined system  $A c = y$ :

$$\begin{bmatrix} f_1(x_1) & \dots & f_n(x_1) \\ f_1(x_2) & \dots & f_n(x_2) \\ \vdots & & \vdots \\ f_1(x_m) & \dots & f_n(x_m) \end{bmatrix} \begin{bmatrix} c_1 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

## Generalizing to arbitrary basis functions

- ... and derive the same normal equations as for line fit

$$A^T A c = A^T y$$

- some examples of basis functions:
  - $\{1, x\}$  .... the line fit from previously
  - $\{1, x, x^2, x^3, \dots, x^k\}$  ..... a polynomial fit
  - $\{x^{-2/3}, x^{2/3}\}$
  - $\{\sin x, \cos x, \sin 2x, \cos 2x, \dots\}$  .... Fourier fit
- the solution  $c$  to the normal equations gives the coefficients of the fitting function
- inverse  $(A^T A)^{-1}$  gives useful statistical information
  - covariances of the fitting parameters  $c$
  - variances  $\sigma^2(c_j)$  on the diagonal

## Arbitrary basis functions: example

- fit data with the basis functions  $\{x^{-1}, x\}$
- Matlab example:
  - load  $(x_i, y_i)$  data from xinvpx.dat
  - design matrix  $a = [1./x \ x]$
  - solve the normal equations for  $(c_1, c_2)$
  - can use the mfile *fitnorm(x,y,Afun)* with ...
  - inline function *Afun=inline('[a./x x]')*

## Solving the normal equations

- $A^T A c = A^T y$  is a linear system
  - Gaussian elimination is sometimes ok and provides the inverse  $(A^T A)^{-1}$  for statistical information
  - LU decomposition is numerically equivalent, and more efficient if the covariance matrix not required
  - Cholesky also an option since  $A^T A$  is positive definite
- all solution methods based on normal equations are inherently susceptible to roundoff error and other numerical problems
- a better approach is to apply decomposition techniques directly to the 'design matrix'  $A$ 
  - QR decomposition is a stable algorithm
  - SVD is best and completely avoids numerical problems

## Normal equations: Numerical issues

- normal equations may be close-to-singular
- very small pivots giving very large  $c_j$ 's that nearly cancel when  $F(x)$  is evaluated
  - data doesn't match the chosen basis functions
  - two of them may be an equally good or equally bad fit
  - $A^T A$  cannot distinguish between the functions so they get similar very large weights
- 'under-determined' due to these ambiguities
- SVD can resolve these problems automatically

## Normal equations: example

- find the least squares solution to the system  $Ac=y$  where  $A = [1 \ -1; 3 \ 2; -2 \ 4]$ ,  $y = [4 \ 1 \ 3]^T$
- $A^T A = [14 \ -3; -3 \ 21]$
- $A^T y = [1 \ 10]^T$
- so normal equations  $A^T A c = A^T y$  are
 
$$\begin{bmatrix} 14 & -3 \\ -3 & 21 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 10 \end{bmatrix}$$
- exact LS solution is  $c_1 = 17/95$ ,  $c_2 = 143/285$

## Normal equations: another example

- find the least squares solution to  $Ac=y$  with
 
$$A = \begin{bmatrix} 3 & -6 \\ 4 & -8 \\ 0 & 1 \end{bmatrix} \quad y = \begin{bmatrix} -1 \\ 7 \\ 2 \end{bmatrix}$$
- normal equations are  $A^T A c = A^T y$  with
 
$$A^T A = \begin{bmatrix} 25 & -50 \\ -50 & 101 \end{bmatrix} \quad A^T y = \begin{bmatrix} 25 \\ -48 \end{bmatrix}$$
- Cholesky factorization is  $A^T A = \begin{bmatrix} 5 & 0 \\ -10 & 1 \end{bmatrix} \begin{bmatrix} 5 & -10 \\ 0 & 1 \end{bmatrix}$
- solution is  $\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 5 \\ 2 \end{bmatrix}$

## Solving the over-determined system

- fit a line through three points (1,1), (2,3), (3,4)
- the over-determined system  $Ac = y$  is
 
$$\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \\ 4 \end{bmatrix}$$
- can solve the normal equations  $A^T A c = A^T y$  and get the fitting function  $y = 1.5x - 0.3333x$
- what about applying Gaussian elimination directly to the over-determined system?
- you get an inconsistent augmented system ....
 
$$\left[ \begin{array}{cc|c} 1 & 1 & 1 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{array} \right]$$

## Why QR factorization?

- why doesn't this approach give the LS solution?
- the elementary row ops applied to A are
 
$$MA = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & -1 \\ 0 & 0 \end{bmatrix}$$
- problem is multiplication by M doesn't preserve the  $L_2$ -norm of the residual:
 
$$\|M(y - Ac)\|_2 \neq \|y - Ac\|_2$$
- so the 'solution' walks away from the LS solution

## Why QR factorization?

- however an orthogonal matrix Q preserves norms:
 
$$\|Qx\|_2 = [(Qx)^T(Qx)]^{1/2} = [x^T Q^T Q x]^{1/2} = [x^T x]^{1/2} = \|x\|_2$$
- so to minimize  $\|y - Ac\|_2$  we can ...
  - look for an orthogonal Q so that ....
  - minimizing  $\|Q^T y - Q^T A c\|_2$  is an easy problem to solve
- factorize the  $m \times n$  matrix  $A = QR$ 
  - $m \times n$  orthogonal Q
  - $n \times n$  upper triangular R
- first how do we find the factorization? ....

## QR factorization

- can apply the Gram-Schmidt process to the columns of A
  - converts a basis  $\{u_1, \dots, u_n\}$  into an orthonormal basis  $\{q_1, \dots, q_n\}$
  - the most direct approach to finding QR
  - not numerically stable though
  - other more sophisticated algorithms are used in practice
- consider a full rank  $n \times n$  matrix A
- the columns of A are
  - linearly independent
  - form a basis of the column space of A
- what is the relationship between  $A = [u_1 | u_2 | \dots | u_n]$  and  $Q = [q_1 | q_2 | \dots | q_n]$ ?

## QR Factorization

- each u can be expressed using the orthonormal basis as:
 
$$u_i = (u_i \cdot q_1)q_1 + (u_i \cdot q_2)q_2 + \dots + (u_i \cdot q_n)q_n \quad i = 1, 2, \dots, n$$
- in matrix form this is

$$[u_1 | u_2 | \dots | u_n] = [q_1 | q_2 | \dots | q_n] \begin{bmatrix} u_1 \cdot q_1 & u_2 \cdot q_1 & \dots & u_n \cdot q_1 \\ u_1 \cdot q_2 & u_2 \cdot q_2 & \dots & u_n \cdot q_2 \\ \vdots & \vdots & \ddots & \vdots \\ u_1 \cdot q_n & u_2 \cdot q_n & \dots & u_n \cdot q_n \end{bmatrix}$$

- $A = QR$
- this is the QR factorization required
- why is R upper triangular?
  - for  $j \geq 2$  the G-S ensures that  $q_j$  is orthogonal to all  $u_1, u_2, \dots, u_{j-1}$

## QR factorization: example

- find the QR decomposition of  $A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix}$
- apply Gram-Schmidt to the columns of A to get columns of Q:
 
$$q_1 = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}, q_2 = \begin{bmatrix} -2/\sqrt{6} \\ 1/\sqrt{6} \\ 1/\sqrt{6} \end{bmatrix}, q_3 = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$
- then  $R = \begin{bmatrix} u_1 \cdot q_1 & u_2 \cdot q_1 & u_3 \cdot q_1 \\ 0 & u_2 \cdot q_2 & u_3 \cdot q_2 \\ 0 & 0 & u_3 \cdot q_3 \end{bmatrix} = \begin{bmatrix} 3/\sqrt{3} & 2/\sqrt{3} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{6} \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$
- so  $A = \begin{bmatrix} 1/\sqrt{3} & -2/\sqrt{6} & 0 \\ 1/\sqrt{3} & 1/\sqrt{6} & -1/\sqrt{2} \\ 1/\sqrt{3} & 1/\sqrt{6} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 3/\sqrt{3} & 2/\sqrt{3} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{6} \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$

## Skinny QR factorization

- suppose A is  $m \times n$  and has rank n (linearly independent columns)
- previous method still works and gives  $A = QR$  with
  - Q  $m \times n$
  - R  $n \times n$
- this is the *economy (skinny) QR factorization*
  - contains all the information necessary to reconstruct A

## Full vs skinny QR factorization

- can also have a full QR factorization with extra stuff
  - $Q$   $m \times m$
  - $R$   $m \times n$
- last  $m-n$  rows of  $R$  are zero
- first  $n$  columns of  $Q$  span the column space of  $A$
- last  $m-n$  columns of  $Q$  span the orthogonal complement of the column space of  $A$ 
  - this is the nullspace of  $A$
  - not needed to solve the LS problem
  - so the skinny QR factorization is good enough for LS problems
- in general if  $A$  has rank  $k < n$  only the first  $k$  columns of  $Q$  are needed

## QR Factorization in Matlab

- the Matlab function  $[Q,R] = qr(A)$  provides the QR factorization of  $A$
- the function  $[Q,R] = qr(A,0)$  provides the skinny QR factorization
  - we'll always use this one
- example:
  - calculate the skinny QR factorization of the  $A$  in the simple 3-point fitting example on slide 23
  - check that the residuals are small

## QR solution to the LS problem

- a solution to the LS problem  $Ac = y$  is obtained by minimizing the 2-norm of the residual
- some simple calculation and apply the QR factorization:
 
$$\begin{aligned} \|y - Ac\|_2 &= \|Q^T(y - Ac)\|_2 \\ &= \|Q^T y - Q^T A c\|_2 \\ &= \|Q^T y - Rc\|_2 \end{aligned}$$
- write the full QR factorization in block matrix form:
 
$$Q = [Q_1 \mid Q_2] \quad R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$$
- then the column vector residual above can be written

$$Q^T y - Rc = \begin{bmatrix} Q_1^T y - R_1 c \\ Q_2^T y - 0 \end{bmatrix}$$

## QR solution to LS problem

- so the 2-norm of the LS residual is
 
$$\|Q^T y - Rc\|_2 = \|Q_1^T y - R_1 c\|_2 + \|Q_2^T y\|_2$$
- magnitude of the residual consists of two parts:
  - the first part can be zero by selecting a suitable  $c$  vector
  - the second part cannot be influenced by the choice of  $c$  so is irrelevant to the LS problem
  - that's why only the skinny QR factorization is needed
  - we'll drop the  $Q_2$  part of  $Q$
- to solve the LS problem  $Ac = y$  choose  $c$  so that
 
$$Q^T y = Rc$$
  - where  $A = QR$  is the skinny QR factorization

## QR, LS, and Matlab

- solve the simple 3-point line fit example on slide 23 using Matlab and the skinny QR factorization
- the backslash operator in Matlab  $A \backslash y$ 
  - if  $A$  rectangular (over-determined) Matlab automatically applies the QR factorization and finds the LS solution
  - Matlab assumes the LS solution is desired when backslash is encountered under this circumstance
  - $Q$  is only used to evaluate  $Q^T y$
  - can avoid storing the  $Q$  matrix by careful algorithm
- for a standard system notated as  $Ax=b$  the LS solution becomes:  $Q^T b = Rx$

## QR vs Cholesky: example

- minimize  $\|Ax - b\|$  with  $A = \begin{bmatrix} 1 & -1 \\ 0 & 10^{-5} \\ 0 & 0 \end{bmatrix}$   $b = \begin{bmatrix} 0 \\ 10^{-5} \\ 1 \end{bmatrix}$
- the normal equations  $A^T A x = A^T b$ 

$$\begin{bmatrix} 1 & -1 \\ -1 & 1 + 10^{-10} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 10^{-10} \end{bmatrix}$$
- have solution  $x_1 = x_2 = 1$
- compare solution to this LS problem with Cholesky and QR keeping 8 significant digits ....

## QR vs Cholesky: example solution

**method 1** (Cholesky factorization)

$A^T A$  and  $A^T b$  rounded to 8 digits:

$$A^T A = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad A^T b = \begin{bmatrix} 0 \\ 10^{-10} \end{bmatrix}$$

no solution (singular matrix)

**method 2** (QR-factorization): factor  $A = QR$  and solve  $Rx = Q^T b$

$$Q = \begin{bmatrix} 1 & -1 \\ 0 & 10^{-5} \\ 0 & 0 \end{bmatrix}, \quad R = \begin{bmatrix} 1 & -1 \\ 0 & 10^{-5} \end{bmatrix}, \quad Q^T b = \begin{bmatrix} 0 \\ 10^{-5} \end{bmatrix}$$

rounding does not change any values

solution of  $Rx = Q^T b$  is  $x_1 = 1, x_2 = 1$

## QR vs normal equations

- in the example Cholesky solution of the normal equations fails due to rounding error
- normal equations can be very inaccurate for ill-conditioned systems where  $\text{cond}(A^T A)$  is large
- but when  $m \gg n$  the normal equations involve
  - half the arithmetic as compared to QR
  - less storage than QR
- if  $A$  is ill-conditioned and ...
  - residual is small then the normal equations are less accurate than QR
  - residual is large then both methods give an inaccurate LS solution
- choosing the right algorithm is not an easy decision

## A third choice: SVD and LS problem

- we'll use the standard notation for the LS problem  $Ax = b$  with  $A$   $m \times n$
- apply the SVD to  $A$  ...
- the norm of the residual is ...
 
$$\begin{aligned} \|r\| &= \|Ax - b\| \\ &= \|USV^T x - b\| \\ &= \|SV^T x - U^T b\| \end{aligned}$$
- minimizing the residual is equivalent to minimizing  $\|Sz - d\|$  where  $z = V^T x$  and  $d = U^T b$

## SVD and LS problem

- written in blocks this is

$$\left\| \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ 0 & 0 & \dots & \sigma_n \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} - \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} \right\|$$

- to choose  $z$  so that  $\|r\|$  is minimal requires ( $k=1, \dots, n$ )
 
$$\begin{aligned} z_k &= d_k / \sigma_k & \sigma_k &\neq 0 \\ z_k &= 0 & \sigma_k &= 0 \end{aligned}$$
- we have  $d = U^T b$  and  $z = V^T x$

## SVD and LS problem: pseudo-inverse

- write  $S^+$  to denote the transpose of the matrix obtained by replacing each non-zero  $\sigma_k$  by its reciprocal
  - this is NOT a regular matrix inverse since  $S$  is not square
- the minimization condition can be written as  $V^T x = S^+ U^T b$  so ...
- the LS solution to  $Ax = b$  (with  $A = USV^T$ ) is
 
$$x = V S^+ U^T b$$
- the matrix  $A^+ = VS^+U^T$  is called the *pseudo-inverse* of the coefficient matrix  $A$ 
  - behaves for rectangular matrices like the normal inverse for square matrices

## SVD and LS problem: sales pitch

- the SVD method is ....
  - powerful
  - convenient
  - intuitive
  - numerically advantageous
- problems with ill-conditioning and large residuals can be circumvented automatically
- the SVD can solve problems for which both the normal equations and QR factorization fail

## SVD and LS problem: zeroing

- use a zero entry in  $S^+$  if  $\sigma_j = 0$  (to machine precision)
- this forces a zero coefficient in the linear combination of basis functions that gives the fitting equation ....
- ... instead of a random large coefficient that has to delicately cancel with another one
- if the ratio  $\sigma_j / \sigma_1 \sim n \varepsilon_m$  then zero the entry in the pseudo-inverse matrix since the value is probably corrupted by roundoff anyway

## Polynomial curve fitting

- consider curve-fitting with monomial basis functions  $\{1, x, x^2, \dots, x^k\}$
- can solve the least-squares problem with any of the previous techniques (normal equations, QR, SVD)
- the simplicity of the basis functions allows some trickery when setting up the equations
  - to fit known data in column vectors  $x$  and  $y$  to the quadratic  $y = c_1 x^2 + c_2 x + c_3$  requires solving the over-determined system

$$\begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots \\ x_n^2 & x_n & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

## Polynomial curve fitting in Matlab

- these types of coefficient matrices are called *Vandermonde matrices*
  - but see interpolation section of this unit ....
- in Matlab:  $A = [x.^2 \ x \ \text{ones}(\text{size}(x))]$ 
  - the least squares solution can then be found with  $x = A \backslash y$
- Matlab can automate this with the *polyfit* function
  - fits data to an arbitrary  $n$ th order polynomial by ...
  - constructing the design matrix  $A$  and ...
  - obtaining the least squares solution by QR factorization
  - vector  $p = \text{polyfit}(x, y, n)$  contains the coefficients of the fitting polynomial in descending order
  - the polynomial can be evaluated at  $xf$  by  $yf = \text{polyval}(p, xf)$
  - it's also possible to analyse residuals and uncertainties with optional parameters to *polyfit* and *polyval* functions

## Interpolation

- general remarks
  - monomial basis functions
  - Lagrange basis
  - Newton basis ... divided differences
  - polynomial wiggle
- piecewise polynomial interpolation
  - cubic splines
  - Bezier curves and B-splines
- Matlab comments

## Interpolation

- interpolation is the 'exact' form of curve-fitting
- for given data points  $(x_i, y_i)$ 
  - curve-fitting finds the solution to the over-determined system that is *closest* to the data (least-squares solution)
  - interpolation finds a function that passes through *all* the points and 'fills in the spaces' smoothly
- piece-wise linear interpolation is the simplest, but lacks smoothness at the *support points*  $(x_i, y_i)$
- to approximate a function outside the range of values of  $x_i$  use *extrapolation*

## Basic ideas

- given: support points  $(x_i, y_i)$   $i = 1, \dots, n$  that are supposed to result from a function  $y = f(x)$
- to find: an interpolating function  $y = F(x)$  valid for a range of  $x$  values that includes the  $x_i$ 's
- requirements
  - $F(x_i) = f(x_i)$ ,  $i = 1, \dots, n$
  - $F(x)$  should be a good approximation of the  $f(x)$
- the function  $f(x)$  may
  - not be known at all
  - not be easy (or possible) to express symbolically
  - not easy to evaluate
  - known only in tabular format



## Basis functions

- $n$  basis functions  $\Phi_1, \Phi_2, \dots, \Phi_n$  can be used to define the interpolating function  

$$F(x) = a_1\Phi_1(x) + a_2\Phi_2(x) + \dots + a_n\Phi_n(x)$$
- polynomial basis functions are common  

$$F(x) = a_1 + a_2x^2 + \dots + a_nx^n$$
- .....so are Fourier interpolations  

$$F(x) = a_1 + a_2e^{ix} + \dots + a_ne^{(n-1)ix}$$
- polynomials are easy to evaluate but there are numerical issues ...

## Monomial basis functions

- $n$  basis functions are  $x^0, x^1, x^2, \dots, x^{n-1}$
- there is a unique polynomial of degree  $n-1$  passing through  $n$  support points
- so no matter how we get the interpolating polynomial it will be unique
- however it can be expressed in multiple ways with different coefficients multiplying the basis functions
  - for instance the *offset monomials*  $(x-a)^0, (x-a)^1, (x-a)^2, \dots, (x-a)^{n-1}$  could be used
  - we develop techniques to use alternative basis functions for the interpolating polynomial (Lagrange, Newton)
- but first look at simple monomials....

## Vandermonde systems

- this is the simple, direct approach to the problem
- example
  - quadratic interpolating polynomial  $y = c_1x^2 + c_2x + c_3$
  - support points  $(x_1, y_1), (x_2, y_2)$  and  $(x_3, y_3)$
  - sub the points into the interpolating function and you get the *Vandermonde system*:

$$\begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

- compare this system to that for curve fitting....

## Vandermonde systems

- $[c_1 \ c_2 \ c_3]$  is supposed to be
  - the *exact, unique* solution to the  $3 \times 3$  non-singular system in interpolation
  - the least squares solution to an  $m \times 3$  over-determined system in curve-fitting
- there is a Matlab function to evaluate the Vandermonde matrix: *vander*( $[y_1 \ y_2 \ y_3]$ )
- but...Vandermonde systems often
  - are ill-conditioned
  - have solutions with very large order of magnitude differences in the coefficients

## Vandermonde systems: example

- yearly prices
 

```
year = [1986 1988 1990 1992 1994 1996];
price = [133.5 132.2 138.7 141.5 137.6 144.2];
A = vander(year);
c = A \ price;
y = linspace(min(year), max(year));
p = polyval(c, y);
plot(year, price, 'o', y, p, '-');
```
- $\text{cond}(A) \sim 10^{31}$ ... not good ☹️
  - serious problems with roundoff error in calculating the coefficients [see the oscillations in the plot]

## Vandermonde systems: example

- coefficients vary over 16 orders of magnitude
- adding and subtracting very large quantities is supposed to give a delicate balance, but the result is mostly roundoff corruption
- a simple re-scaling using offset monomials can sometimes fix the problem
 

```
ys = year - mean(year);
A = vander(ys);
```
- system not ill-conditioned now 😊
- coefficients vary over only 5 orders of magnitude
  - no spurious oscillations now from roundoff

## Lagrange polynomials

- an alternative basis for polynomials of degree n
- first degree polynomial first...
- the (linear) poly passing through  $(x_1, y_1)$  &  $(x_2, y_2)$  is:

$$P_1(x) = y_1 \underbrace{\frac{x - x_2}{x_1 - x_2}}_{L_1} + y_2 \underbrace{\frac{x - x_1}{x_2 - x_1}}_{L_2}$$

- find this representation by ...
  - writing the Vandermonde system
  - solving for  $c_1$  and  $c_2$  and ...
  - re-arranging the polynomial in the form above

## Lagrange polynomials

- now the interpolating polynomial is expressed as  $p_1(x) = y_1 L_1(x) + y_2 L_2(x)$
- the basis functions  $L_1(x)$  &  $L_2(x)$  are called first-degree *Lagrange interpolating polynomials*
- continuing to second degree we get...

$$P_2(x) = y_1 \underbrace{\frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)}}_{L_1(x)} + y_2 \underbrace{\frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)}}_{L_2(x)} + y_3 \underbrace{\frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)}}_{L_3(x)}$$

## Lagrange polynomials

- in general for nth order interpolation  

$$p_{n-1}(x) = y_1 L_1(x) + y_2 L_2(x) + \dots + y_n L_n(x)$$
 where....
- the nth degree *Lagrange interpolating polynomials* are

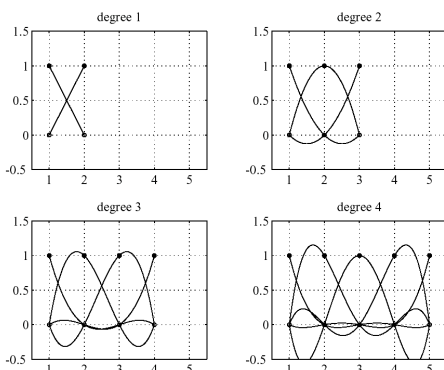
$$L_j(x) = \prod_{k=1, k \neq j}^n \frac{x - x_k}{x_j - x_k}$$

- *notation warning*: the meaning of the symbol ' $L_j(x)$ ' depends on the degree of interpolating polynomial being used

## Lagrange polynomials

- no system of equations has to be solved to get the interpolating polynomial with Lagrange polynomial basis functions
- not susceptible to roundoff error problems
- illustrative Matlab function *lagrint* shows an efficient implementation of Lagrange polys

## Lagrange polynomials



## Lagrange polynomials

- both Vandermonde and Lagrange can be improved on
  - too much arithmetic involved
  - data points cannot be added or deleted without starting the calculations again from scratch
  - we don't know what degree polynomial to use up front and we can't adjust that later without starting again
- an alternative is ....

## Newton basis functions

- Newton basis functions are  $1, (x-x_1), (x-x_1)(x-x_2), (x-x_1)(x-x_2)(x-x_3), \dots, (x-x_1)(x-x_2)\dots(x-x_n)$
- express the interpolating polynomial  $p_n(x)$  in terms of this basis:

$$P_n(x) = c_1 + c_2(x-x_1) + c_3(x-x_1)(x-x_2) + \dots + c_{n+1}(x-x_1)(x-x_2)\dots(x-x_n)$$

- Newton basis functions
  - are computationally efficient
  - have important relevance in numerical integration
  - have good numerical properties

## Newton basis functions

- first consider the quadratic version...

$$p_2(x) = c_1 + c_2(x-x_1) + c_3(x-x_1)(x-x_2)$$

- apply the support point constraints  $p_n(x_i) = y_i$

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & (x_2-x_1) & 0 \\ 1 & (x_3-x_1) & (x_3-x_1)(x_3-x_2) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

- and apply forward elimination, first to get

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & (x_3-x_2) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ \frac{y_2-y_1}{x_2-x_1} \\ \frac{y_3-y_1}{x_3-x_1} \end{bmatrix}$$

## ...First order divided differences

- this can be written compactly in the form

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & (x_3-x_2) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ f[x_1, x_2] \\ f[x_1, x_3] \end{bmatrix}$$

- where  $f[x_1, x_2]$  is a *first order divided difference*

$$f[x_i, x_j] = \frac{y_j - y_i}{x_j - x_i}$$

- continuing with the elimination we get...

## ...Second order divided differences

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ f[x_1, x_2] \\ f[x_1, x_2, x_3] \end{bmatrix}$$

- where  $f[x_1, x_2, x_3]$  is a *second order divided difference*

$$f[x_1, x_2, x_3] = \frac{f[x_2, x_3] - f[x_1, x_2]}{x_3 - x_1}$$

- in general, for  $n$ th degree poly interpolation we get...

## ....nth order divided differences

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_{n+1} \end{bmatrix} = \begin{bmatrix} f[x_1] \\ f[x_1, x_2] \\ f[x_1, x_2, x_3] \\ \vdots \\ f[x_1, x_2, \dots, x_{n+1}] \end{bmatrix}$$

- where  $f[x_1, x_2, \dots, x_n]$  is an *nth order divided difference*

$$f[x_1, x_2, \dots, x_n] = \frac{f[x_2, \dots, x_n] - f[x_1, \dots, x_{n-1}]}{x_n - x_1}$$

- notation warning*: the indices usually start at zero, but here they are adjusted to be consistent with Matlab convention .... array indices cannot be zero

## Divided differences

- find the 3rd degree Newton interpolating poly for first four data points in the table below

$x_i$	$y_i$	$f[x_i, x_{i+1}]$	$f[x_i, \dots, x_{i+2}]$	$f[x_i, \dots, x_{i+3}]$	$f[x_i, \dots, x_{i+4}]$
3.2	22.0	8.400	2.856	-0.528	0.256
2.7	17.8	2.118	2.012	0.865	
1.0	14.2	6.342	2.263		
4.8	38.2	16.750			
5.6	51.7				

- divided differences can be calculated as shown

$$p_3(x) = 22.0 + 8.400(x-3.2) + 2.856(x-3.2)(x-2.7) - 0.528(x-3.2)(x-2.7)(x-1.0)$$

## Adding a data point is easy

- to find the 4th degree poly that fits all the five points in the table
  - calculate the extra divided difference(s) and get the last coefficient (see the table on previous slide)
  - you start with  $p_3(x)$  and add one term to it

$$p_4(x) = p_3(x) + 0.256(x - 3.2)(x - 2.7)(x - 1.0)(x - 4.8)$$

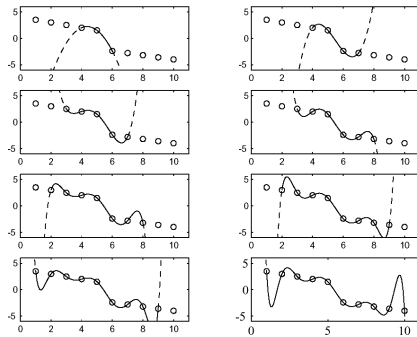
- data points can easily be added or deleted
- a better form for computation is with nested multiplication (Horner's rule):

$$p_3(x) = ((-0.528(x - 1.0) + 2.856)(x - 2.7) + 8.400)(x - 3.2) + 22.0$$

## Wiggle

- more support points  $\Rightarrow$  higher degree interpolating polynomial  $F(x)$  is required
- $F(x_i) = y_i$  is OK since the interpolant passes through all the support points
- but higher order polynomials will exhibit rapid oscillations between the support points
- this polynomial wiggle is an extraneous artifact of the interpolation method
- limits the applicability of higher order polynomial interpolation to improve accuracy
- suggests piecewise methods....

## Wiggle



## Piecewise polynomial interpolation

- instead of finding a single higher order interpolating polynomial passing through all the support points...
- ...find multiple lower order polynomials going through subsets of support points
- the joints where these fit together are called **breakpoints** or **knots**
- desire for global performance raises complexity by demanding constraints on how the local interpolants relate to their neighbours

## Continuity constraints

- can demand  $f(x)$ ,  $f'(x)$  and/or  $f''(x)$  to be continuous at the breakpoints
- fundamental issue: are neighbouring interpolating polynomials constrained with respect to each other? ...
  - leads to large, sparse systems to solve (cubic splines)
- ... or with respect to the original function?
  - leads to de-coupled equations to solve, but you need more information from the data points (Hermite)
  - de-coupled polynomials require identification of the appropriate sub-interval for evaluation

## Searching for sub-intervals

- $p_j(x)$  is the interpolating polynomial for the  $j$ th sub-interval  $(x_j, x_{j+1})$
- how to locate the sub-interval which brackets a given test point  $x$ ?
- assume the data is ordered or manage appropriate book-keeping to order it
- two techniques that work:
  - incremental search ... look through the data in sequence until the bracketing interval is found
  - binary search ... use bisection to locate the sub-interval that  $x$  lies in

## Piecewise interpolants

- piecewise linear on sub-intervals
  - solve for coefficients using Lagrange interpolating polynomials
- piecewise quadratic: conic splines
  - exact representation of lines, circle, ellipses, parabolas and hyperbolas
- piecewise cubic: cubic splines
- what's a spline?
  - carries some element of slope or curve shape constraint
  - represent the curve of minimum strain energy (abstraction of beam theory, e.g.  $f'''' = 0$  at break points)
  - drafting device from old times

## Why cubic splines?

- piecewise linear interpolation provides....
  - a smooth  $y'(x)$  everywhere and...
  - zero  $y''(x)$  inside the sub-intervals but...
  - undefined (or infinite)  $y''(x)$  at the breakpoints  $x_j$
- cubic splines improve the behaviour of  $y''(x)$  ....

## Constructing cubic splines

- consider  $n$  tabulated support points
 
$$y_j = y(x_j), j = 1, 2, \dots, n$$
- first use *linear* interpolation on the  $j$ th sub-interval  $(x_j, x_{j+1})$
- the local interpolant is
 
$$y = F(x) = Ay_j + By_{j+1} \quad \dots \text{eqn 1}$$
 with coefficients
 
$$A \equiv \frac{x_{j+1} - x}{x_{j+1} - x_j} \quad B \equiv 1 - A = \frac{x - x_j}{x_{j+1} - x_j}$$
 derived from Lagrange interpolating polynomials

## Constructing cubic splines

- suppose (blindly for now) that we have tabulated values for the second derivative at each breakpoint  $y_j''(x_j)$
- add to the RHS of eqn [1] a cubic polynomial so
  - $y = Ay_j + By_{j+1} + p(x)$
- to ensure that this doesn't alter continuity at the breakpoints we have to have
  - $p(x_j) = p(x_{j+1}) = 0$
- to ensure that the second derivative is continuous at the breakpoints we have to have
  - $y''$  varying linearly (i.e. IS linear) from  $y_j''$  to  $y_{j+1}''$
- can we do all this?

## Constructing cubic splines

- YES ... and to make it work we have to have
 
$$y = Ay_j + By_{j+1} + Cy_j'' + Dy_{j+1}''$$

$$C \equiv \frac{1}{6}(A^3 - A)(x_{j+1} - x_j)^2$$

$$D \equiv \frac{1}{6}(B^3 - B)(x_{j+1} - x_j)^2$$
- the A, B, C, D factors depend on  $x$ :
  - A, B are linearly dependent on  $x$  (from the previous expressions) and ...
  - C, D are cubically dependent on  $x$  (through A, B)

## Constructing cubic splines

- calculate the derivatives and check that it works
 
$$\frac{dy}{dx} = \frac{y_{j+1} - y_j}{x_{j+1} - x_j} - \frac{3A^2 - 1}{6}(x_{j+1} - x_j)y_j'' + \frac{3B^2 - 1}{6}(x_{j+1} - x_j)y_{j+1}''$$
- this eqn [2] comes from the derivatives
 
$$\frac{dA}{dx} = \frac{-1}{x_{j+1} - x_j}$$

$$\frac{dB}{dx} = \frac{1}{x_{j+1} - x_j}$$

$$\frac{dC}{dx} = \frac{1}{6}(3A^2 - 1)\frac{dA}{dx}(x_{j+1} - x_j)^2 = -\frac{1}{6}(3A^2 - 1)(x_{j+1} - x_j)$$

$$\frac{dD}{dx} = \frac{1}{6}(3B^2 + 1)\frac{dB}{dx}(x_{j+1} - x_j)^2 = \frac{1}{6}(3B^2 + 1)(x_{j+1} - x_j)$$

## Constructing cubic splines

- the second derivative is

$$\frac{d^2y}{dx^2} = -\frac{d}{dx} \left( \frac{3A^2 - 1}{6} \right) (x_{j+1} - x_j) y_j'' + \frac{d}{dx} \left( \frac{3B^2 - 1}{6} \right) (x_{j+1} - x_j) y_{j+1}''$$

$$= A y_j'' + B y_{j+1}''$$

- A = 1 and B = 0 when  $x = x_j$  and opposite for  $x_{j+1}$   
so  $y''(x_j) = y_j''$  and  $y''(x_{j+1}) = y_{j+1}''$
- this ensures that
  - the second derivative actually agrees with the tabulated assumed values
  - the continuity condition for the second derivatives at the breakpoints is satisfied
- so now what do we do about our assumed  $y_j''$ ??

## Constructing cubic splines

- we now get an equation to solve for these unknown (assumed)  $y_j''$  values
- the trick is to demand continuity of the first derivative at the breakpoints
- use eqn [2] to evaluate it at
  - $x = x_j$  the right endpoint of  $(x_{j-1}, x_j)$ , and
  - $x = x_j$  the left endpoint of  $(x_j, x_{j+1})$  and
  - equate these two for continuity
- after some [messy] simplification you get the n-2 **cubic spline equations** ( $j = 2, \dots, n-1$ ) [eqn 3]

$$\frac{x_j - x_{j-1}}{6} y_{j-1}'' + \frac{x_{j+1} - x_{j-1}}{3} y_j'' + \frac{x_{j+1} - x_j}{6} y_{j+1}'' = \frac{y_{j+1} - y_j}{x_{j+1} - x_j} - \frac{y_j - y_{j-1}}{x_j - x_{j-1}}$$

## Cubic spline equations!

$$\begin{bmatrix} h_1 & 2(h_1 + h_2) & h_2 & & & \\ & h_2 & 2(h_2 + h_3) & h_3 & & \\ & & & \ddots & & \\ & & & & h_{n-2} & 2(h_{n-2} + h_{n-1}) & h_{n-1} \end{bmatrix} \begin{bmatrix} y_1'' \\ y_2'' \\ y_3'' \\ \vdots \\ y_{n-1}'' \end{bmatrix} = 6 \begin{bmatrix} f[x_2, x_3] - f[x_1, x_2] \\ f[x_3, x_4] - f[x_2, x_3] \\ \vdots \\ f[x_{n-2}, x_{n-1}] - f[x_{n-3}, x_{n-2}] \end{bmatrix}$$

- $h_j = x_{j+1} - x_j, j = 1, 2, \dots, n-1$   
is the size of the  $j$ th interval

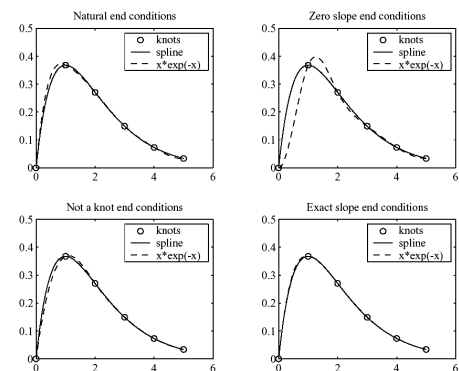
## Cubic spline equations

- these are n-2 equations in the n unknown breakpoint second derivatives  $y_j'', j = 1, \dots, n$
- there is a two parameter family of solutions unless we specify additional constraints
- for a unique solution we can specify boundary conditions at the endpoints  $x_1$  and  $x_n$ 
  - defines the behaviour of the interpolating function at the global endpoints
- three choices are common for cubic spline boundary conditions ....

## Cubic splines: boundary conditions

- $y_1'' = y_n'' = 0$ , i.e. a smooth flow away from the two global endpoints (these called **natural** cubic splines) OR
- set  $y_1'$  and/or  $y_n'$  to values calculated from eqn [2] so that  $y_1'$  and/or  $y_n'$  have desired values (**specified endpoint slopes**)
- force continuity of the third derivative at the first and last breakpoints, e.g.  $y_2'''$  from first or second interval is to be the identical value, similarly  $y_{n-1}'''$ 
  - this is called the **not-a-knot condition**
  - it effectively makes the first two interpolating cubics identical

## Cubic splines: boundary conditions



## Cubic splines: computational issues

- have to solve a linear system for the  $n$  unknowns  $y_j''$  consisting of
  - $n-2$  spine equations
  - two boundary conditions
- this is a (sparse) tri-diagonal linear system
- only the main diagonal and its neighbours have non-zero entries
- this reflects the fact that each sub-interval in the interpolation problem is coupled only to its two nearest neighbours
- special efficient algorithms are available for solving tri-diagonal systems

## Cubic splines: example

- find the equations for the four natural cubic splines which interpolate the data points:
  - $(-2,4)$ ,  $(-1,-1)$ ,  $(0,2)$ ,  $(1,1)$ ,  $(2,8)$
- all  $h_j = x_{j+1} - x_j = 1$  for this data [nice]
- the spline equations

$$\frac{h_j}{6}y_{j-1}'' + \frac{h_{j+1} + h_j}{3}y_j'' + \frac{h_{j+1}}{6}y_{j+1}'' = \frac{y_{j+1} - y_j}{h_{j+1}} - \frac{y_j - y_{j-1}}{h_j}$$

are ( $j = 2,3,4$ ):

$$\frac{1}{6}y_{j-1}'' + \frac{2}{3}y_j'' + \frac{1}{6}y_{j+1}'' = y_{j+1} - 2y_j + y_{j-1}$$

## Cubic splines: example (cont)

- written out this system is

$$j = 2: \frac{1}{6}y_1'' + \frac{2}{3}y_2'' + \frac{1}{6}y_3'' = y_3 - 2y_2 + y_1$$

$$j = 3: \frac{1}{6}y_2'' + \frac{2}{3}y_3'' + \frac{1}{6}y_4'' = y_4 - 2y_3 + y_2$$

$$j = 4: \frac{1}{6}y_3'' + \frac{2}{3}y_4'' + \frac{1}{6}y_5'' = y_5 - 2y_4 + y_3$$

- natural splines have  $y_1'' = y_5'' = 0$  so the system simplifies to:

$$4y_2'' + y_3'' = 48$$

$$y_2'' + 4y_3'' + y_4'' = -24$$

$$y_3'' + 4y_4'' = 48$$

solution

$$\begin{aligned} y_1'' &= 0 \\ y_2'' &= 15.4286 \\ y_3'' &= -13.7143 \\ y_4'' &= 15.4286 \\ y_5'' &= 0 \end{aligned}$$

## Cubic splines: example (cont)

- step #1 is complete now we have the second derivatives at the breakpoints
- now use these values to obtain the cubic spline equation coefficients  $A, B, C, D$  [formulas on slides 75&77], with  $j=1, \dots, 4$
- first  $j = 1$ :

$$A = x_2 - x = -(1 + x)$$

$$B = 1 - A = x + 2$$

$$C = \frac{1}{6}(A^3 - A) = \frac{1}{6}[-(1+x)^3 + (1+x)]$$

$$D = \frac{1}{6}(B^3 - B) = \frac{1}{6}[(x+2)^3 - (x+2)]$$

## Cubic splines: example (cont)

- the spline equation for the first interval  $-2 < x < -1$  is then given by

$$\begin{aligned} y &= Ay_1 + By_2 + Cy_1'' + Dy_2'' \\ &= -(1+x)(4) + (x+2)(-1) + 0 + \frac{1}{6}[(x+2)^3 - (x+2)](15.4286) \\ &= 2.57(x+2)^3 - 4(x+1) - 3.57(x+2) \quad \dots S1 \end{aligned}$$

- $j = 2$  gives the spline equation for the second interval  $-1 < x < 0$

$$A = x_3 - x = -x$$

$$B = 1 - A = x + 1$$

$$C = \frac{1}{6}(A^3 - A) = \frac{1}{6}[-x^3 + x]$$

$$D = \frac{1}{6}(B^3 - B) = \frac{1}{6}[(x+1)^3 - (x+1)]$$

## Cubic splines: example (cont)

$$\begin{aligned} y &= Ay_2 + By_3 + Cy_2'' + Dy_3'' \\ &= -x(-1) + (x+1)(2) + \frac{1}{6}[-x^3 + x](15.4286) + \frac{1}{6}[(x+1)^3 - (x+1)](-13.7143) \\ &= -2.57x^3 - 2.29(x+1)^3 + 3.57x + 4.29(x+1) \quad \dots S2 \end{aligned}$$

- for the third interval  $0 < x < 1$  we have  $j = 3$ :

$$A = x_4 - x = 1 - x$$

$$B = 1 - A = x$$

$$C = \frac{1}{6}(A^3 - A) = \frac{1}{6}[(1-x)^3 - (1-x)]$$

$$D = \frac{1}{6}(B^3 - B) = \frac{1}{6}[x^3 - x]$$

and the third spline equation ....

### Cubic splines: example (cont)

$$\begin{aligned}
 y &= Ay_3 + By_4 + Cy_3'' + Dy_4'' \\
 &= (1-x)(2) + x(1) + \frac{1}{6}[(1-x)^3 - (1-x)](-13.7143) + \frac{1}{6}[x^3 - x](15.4286) \\
 &= -2.29(1-x)^3 + 2.57x^3 + 4.29(1-x) - 1.57x \quad \dots \text{S3}
 \end{aligned}$$

- finally, for the 4th interval  $1 < x < 2$  we have  $j = 4$ :

$$A = x_5 - x = 2 - x$$

$$B = 1 - A = x - 1$$

$$C = \frac{1}{6}(A^3 - A) = \frac{1}{6}[(2-x)^3 - (2-x)]$$

$$D = \frac{1}{6}(B^3 - B) = \frac{1}{6}[(x-1)^3 - (x-1)]$$

and the fourth spline equation ....

### Cubic splines: example (cont)

$$\begin{aligned}
 y &= Ay_4 + By_5 + Cy_4'' + Dy_5'' \\
 &= (2-x)(1) + (x-1)(8) + \frac{1}{6}[(2-x)^3 - (2-x)](15.4286) + 0 \\
 &= 2.57(2-x)^3 - 1.57(2-x) + 8(x-1) \quad \dots \text{S4}
 \end{aligned}$$

- these equations (S1-S4) are the four natural cubic spline equations for  $y$  over the interval  $-2 < x < 2$
- to evaluate  $y(x)$  you decide which interval  $x$  lies in and use the applicable equation

### Font wars

- proportional fonts are rendered at any size using curves determined by interpolation through specified points
- the curves are rasterized for display following 'hints' to keep the fonts realistic in small sizes
- Type I fonts, Adobe 1985
  - used in postscript and acrobat
  - based on cubic splines as developed above
- TrueType fonts, Apple 1988 + now MS
  - conic splines
  - a subset of cubic splines with simpler interpolation
  - faster rendering but require more 'hints'

### Interpolation: Matlab implementation

- the basic Matlab functions you need to know are
  - interp1*: one-dimensional interpolation with piecewise polynomials
  - spline*: one-dimensional interpolation with cubic splines using not-a-knot or fixed-slope end conditions
- there are others too
  - multi-dimensional interpolations
  - a sophisticated spline toolbox

### Interpolation: Matlab implementation

- ytest = interp1(x,y,xtest,method)**
  - $y$  = tabulated function values
  - $xtest$  = test  $x$  value to evaluate the interpolant
  - $x$  = tabulated  $x$  values for interpolation (1:n default)
  - method = 'nearest' [nearest neighbour constant], 'linear', 'cubic' [cubic polys s.t. interpolant & first derivative are continuous at the breakpoints], or 'spline' [cubic splines, same as spline function]
  - ytest = calculated interpolated value corresponding to  $xtest$
- default for splines is not-a-knot end conditions
- if  $\text{size}(y) = \text{size}(x)+2$ , first and last elements are used for  $y'(x_1)$  and  $y'(x_n)$  end slopes