# From Functional Data to Smooth Functions

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- We need a flexible method for constructing functions from noisy discrete data.
- The method should be able to reproduce any feature that interests us in a function, no matter how complicated.
- The computation should be reasonably fast, even when tens or hundreds of thousands of discrete values are available.
- In this talk, we consider the most popular technique, *basis function expansions*.

- We describe two basis function systems in detail:
  - Fourier bases
  - B-spline bases
- as well as some other important systems.
- We also ask about how to estimate derivatives,
- including a bad idea.

# Outline

- A basis function system is a set of $K$ known functions $\phi_k(t)$ that are:
  - linearly independent of each other
  - can be extended to include any number $K$ in the system
- A function $x(t)$ is constructed as a linear combination of these basis functions:

$$x(t) = \sum_{k=1}^{K} c_k \phi_k(t)$$

- If vector $\mathbf{c}$ contains the coefficients, and the vector $\phi$ contains the basis functions, then

$$x(t) = \mathbf{c}' \phi(t).$$

# Basis function systems and derivatives

- In principle, computing derivatives is easy:

$$D^m x(t) = \sum_{k=1}^{K} c_k D^m \phi_k(t)$$

- but not all basis functions have derivatives that behave reasonably, or can even be calculated.

# The monomial basis

- Polynomials are perhaps the oldest and best known basis function expansion.
- A polynomial is the form

$$x(t) = \sum_{k=1}^{K} c_k t^{k-1}.$$

- The basis functions are the *monomials*: $1, t, t^2, t^3, \ldots$
- Polynomials can work fine for simple problems only requiring $K = 5$ or so, but have severe problems tracking sharp localized features, and can run into computational problems for unequally spaced data.

# Polynomials and derivatives

- Derivative estimation is a big problem for polynomials because their derivatives become less and less complex, the higher the order of derivative.
- For a polynomial of degree $m$, the derivative of order $m+1$ is zero.
- But in most real–world systems, derivatives become more complex as the order of the derivative increases.

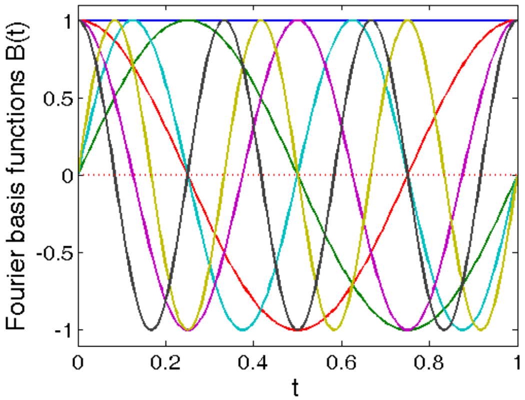
# Outline

- The basis functions are sine and cosine functions of increasing frequency:

$$1, \sin(\omega t), \cos(\omega t), \sin(2\omega t), \cos(2\omega(t), \ldots$$

$$\sin(m\omega t), \cos(m\omega(t), \ldots$$

- The constant $\omega$ defines the period of oscillation of the first sine/cosine pair. This is $\omega = 2\pi/P$ where $P$ is the period.
- $K = 2M + 1$ where $M$ is the largest number of oscillations in period $P$ that are required.


Fourier basis functions B(t)
1
0.5
0
-0.5
-1
0
0.2
0.4
0.6
0.8
1
t

# Advantages of Fourier basis functions

- Fourier bases were the only alternative to monomial bases until the middle of the 20th century.
- They have excellent computational properties, especially if the times of observation are equally spaced.
- They are natural for describing data which are periodic, such as the annual weather data, gait cycle data and so on.
- Their periodicity is a problem, however, for nonperiodic data, such as the growth curves.
- But the Fourier basis is still the first choice in many fields, such as signal analysis, even when the data are not periodic.

# Fourier bases and derivatives

- Computing derivatives is easy since

$$D\sin(\omega t) = \omega\cos(\omega t)$$

$$D\cos(\omega t) = -\omega\sin(\omega t)$$

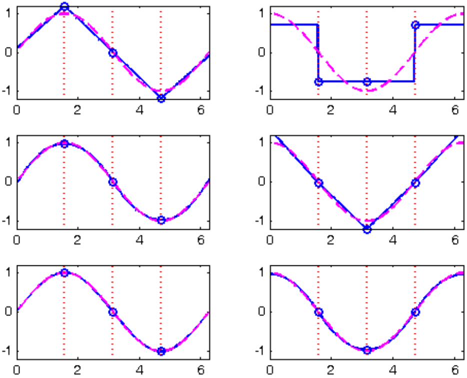
- We say that this system is closed under differentiation; the derivative of a Fourier series expansion is also a Fourier series expansion.
- The Fourier series is infinitely differentiable.

# Outline

- Splines are polynomial segments joined end-to-end.
- The segments are constrained to be smooth at the join.
- The values of $t$ at which adjacent segments are joined are called *knots*.
- The *order* $m$ (order = degree + 1) of the polynomial segments and
- the location of the knots define the spline basis system.

# An example of spline functions

- The following figure shows splines of three orders, each with three knot values.
- The splines are defined so as to offer the best fit to a sine function, shown in the left panels.
- How well the derivatives of these splines fit the derivative of the sine, the cosine, is shown in the right panels.



1
0
-1
0
2
4
6

# Derivatives and splines

- Because splines are constructed from polynomials, computing their derivative at any point between two knots is simple. There, the highest nontrivial order of derivative is $m - 1$ for order $m$ splines.
- At a knot, it is usual to require that the derivatives up to order $m - 2$ also join. That is, the derivative of order $m - 2$ of a spline function is usually *continuous*.
- The most popular choice of order is 4, implying continuous second derivatives. The second derivatives have straight line segments.

# Spline functions and degrees of freedom

- How can we quantify the flexibility of a spline function of order $m$?
- In the usual case, there are $m - 1$ constraints on the adjacent polynomials, corresponding to the requirement that $m - 2$ derivatives plus the function values are required to match at the knot.
- Given the first segment, with $m$ degrees of freedom, this means that we gain one degree of freedom with each knot to the right of the first segment.
- The total number of degrees of freedom is

$$order\ m\ +\ number\ of\ interior\ knots$$

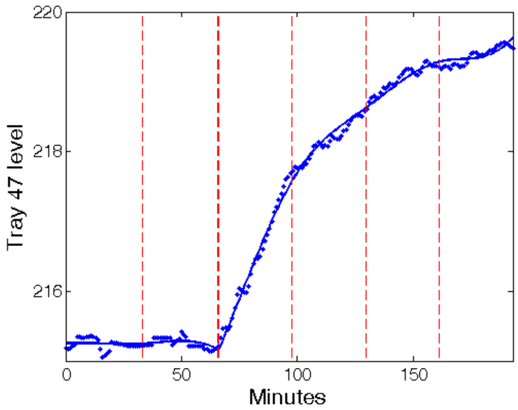
# How are knots chosen?

- Knots are often spaced equally.
- But two important rules should be observed in placing knots:
  - Place more knots where you know there is strong curvature, and fewer where the function changes slowly.
  - But be sure that there is at least one data point in any interval.
- Later, we will consider placing a knot at each point of observation.

# Spline functions and coincident knots

- Sometimes we need less smoothness at a specific point.
- For example, we will see problems where a function needs to be continuous at a point, but its derivative is discontinuous.
- When multiple knots are placed at the same point, the convention is that a spline loses one derivative for each additional knot.
- An order 4 spline with 3 coincident knots is continuous at that point, but does not have a first derivative.
- An order 4 spline with 4 coincident knots is discontinuous at that point.

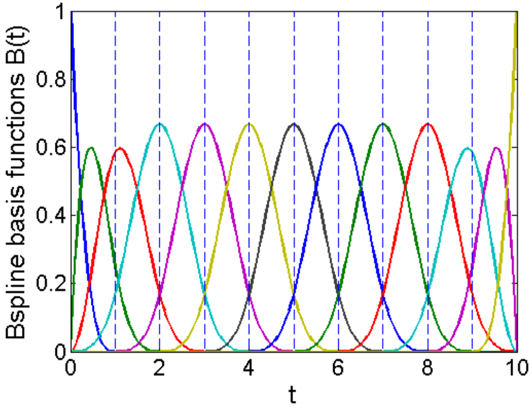
There are three coincident knots at the second location for the refinery data to permit a discontinuous first derivative.



# The B-spline basis system

- Any spline function with $K$ degrees of freedom can be expressed as a linear combination of $K$ basis spline functions .
- Among many possibilities, the B-spline system, developed in the 1940's, is the most popular.
- B-spline basis functions are themselves spline functions.
- Any B-spline basis function is positive over at most $m$ adjacent intervals.
- This ensures that computation is fast for even tens of thousands of basis functions.

# 13 order 4 B-spline basis functions



# Outline

- Basis systems can be constructed in many other ways:

  **Power Basis:** $t^{\lambda_1}, t^{\lambda_2}, t^{\lambda_3}, \ldots$ where the powers are distinct but not necessarily integers or even positive.

  **Exponential Basis:** $e^{\lambda_1 t}, e^{\lambda_2 t}, e^{\lambda_3 t}, \ldots$ where the $\lambda$'s are distinct.

## Wavelet bases

- A recent development, wavelet bases combine some of the advantages of both Fourier and B-spline bases.
- They are especially good at tracking sharp highly localized features,
- and separating a signal into components which reflect both specific frequencies and specific locations on the $t$-axis.
- Because of their computational efficiency, they are often used for image compression.
- For example, the FBI uses wavelets to store fingerprint information.

# The constant basis

Let's not neglect the simplest basis system of all: consisting of a single basis function $\phi_1(t) = 1$. We often need to fit a constant to data.

# Empirical basis functions

- We will look at functional *principal components analysis* later.
- This is essentially a method for estimating orthogonal basis functions from functional data that capture as much of the variation as possible given a fixed number of basis functions $K$.

# Designer or customized basis functions

- Later, when we come to differential equation models, we will see how to tailor a basis system to the known characteristics of a set of data.
- Designer bases like these can be much more efficient at representing functional variation.

# Outline

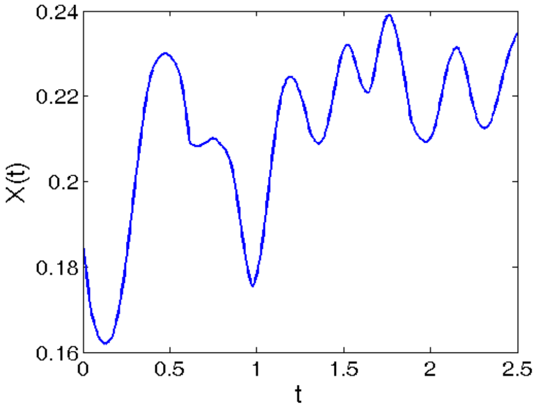
- It is common practice to estimate a derivative by taking the difference between adjacent function values divided by the difference between adjacent time values:

$$\Delta x(t_i) = \frac{x(t_{i+1}) - x(t_i)}{t_{i+1} - t_i}$$

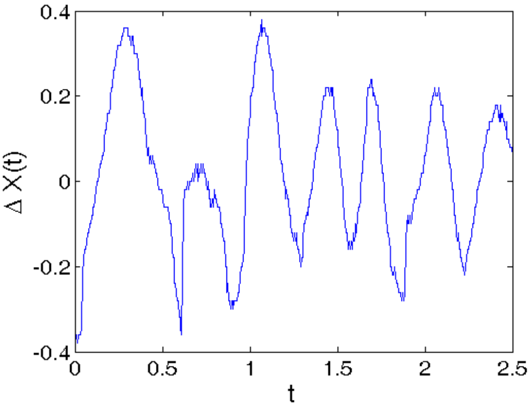
- The second derivative can be estimated by applying this differencing process to the first difference ratios.
- This only works for very smooth functions observed without appreciable error.
- Even the smallest amount of error is greatly magnified by differencing.

- The following displays show what happens when we difference a record of pen position that has a signal-to-noise ratio of 500-to-1, and which is sampled 200 times per second.
- The third order difference ratios are virtually worthless as an estimates of the values of the third derivative, which we will need in later analyses.

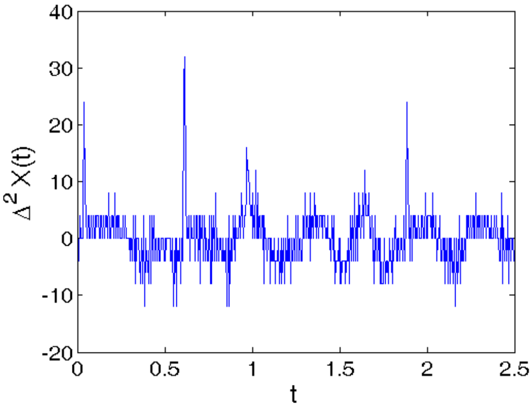
# The pen position function



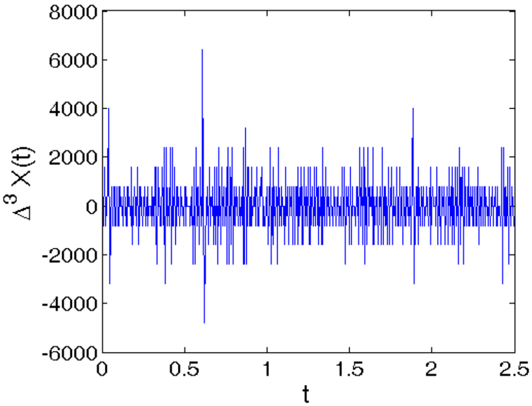
# The first difference ratios



# The second difference ratios



# The third difference ratios



# Where we go from here

- Now we need to see how to fit a basis function expansion to noisy data.
- The simplest process is through least squares approximation.
- This is essentially the use of multiple regression analysis, where the covariates are the basis function values corresponding to time sampling points.
- This works reasonably well, but we will see how to do even better later.

# Outline

- Controlling smoothness by limiting the number of basis functions is discontinuous; roughness penalties allow continuous control over smoothness.
- We want to be able to define “smooth” in ways that are appropriate to our problems.
  - We may want a smooth derivative rather than just a smooth function.
  - What is smooth in one situation is not smooth in another. Smoothness has to be defined differently for periodic functions, for example.
- We find that roughness penalty smoothing gives better results.
- Roughness penalties are connected to fitting data by a differential equation; they are models for process dynamics.

# Outline

We have two competing objectives:

1. Fit the data well; keep bias low.
2. Keep the fit smooth so as to
   - filter out noise
   - get better estimates of derivatives

$$\textit{Mean squared error} = \textit{Bias}^2 + \textit{Sampling Variance}$$

We can often greatly reduce MSE by trading a little bias off against a lot of sampling variance.

# Quantifying roughness

- **The classic: curvature in the function**

$$\mathrm{PEN}_2(x) = \int [D^2 x(s)]^2 \, ds \, .$$

$[D^2 x(s)]^2$ measures the *squared curvature* in $x$ at $s$. This penalty measures *total squared curvature*.

- **Curvature in acceleration:**

$$\mathrm{PEN}_4(x) = \int [D^4 x(s)]^2 \, ds$$

- These two penalties also define what we mean by "smooth"; any function that has zero penalty is "hyper–smooth." A straight line for the classic, a cubic polynomial for the acceleration penalty.

# Harmonic acceleration

- If the process is periodic, it is natural to think of a *constant* $+$ *sinusoid* as "hyper–smooth".
- This suggests that we use

$$\mathrm{PEN}_H(x) = \int [D^3 x(s) + \omega^2 Dx(s)]^2 \, ds$$

  where $2\pi/\omega$ is the period.
- The functions $1$, $sin(\omega t)$, and $\cos(\omega t)$ all have zero penalties, as does any linear combination of them.

# Some questions to think about

- Writing $Lx(s) = D^3x(s) + \omega^2 Dx(s)$, we have

$$\mathrm{PEN}_H(x) = \int [Lx(s)]^2 \, ds$$

- Can we think of other *differential operators* $L$ that might be useful?
- If we have a small number of “hyper–smooth” functions in mind, can we find a differential operator $L$ that will assign zero penalty to them?
- Can use the data themselves to tell us something about the right differential operator $L$?

# Outline

- Notation:
  - $\mathbf{y}$ is the $n$-vector of data $y_j$ to be smoothed.
  - $\mathbf{t}$ is the $n$-vector of values of $t_j$.
  - $\mathbf{W}$ is a symmetric positive definite weight matrix.
  - $x(\mathbf{t})$ is the $n$-vector of fitted values, and $x(t)$ has the basis function expansion

$$x(t) = \sum_k^K c_k \phi_k(t) = \mathbf{c}' \phi(t)$$

- The penalized least squares criterion is

$$\mathrm{PENSSE}_\lambda(x|\mathbf{y}) = [\mathbf{y} - x(\mathbf{t})]' \mathbf{W} [\mathbf{y} - x(\mathbf{t})] + \lambda \, \mathrm{PEN}(x) \; ,$$

# How the smoothing parameter works

*Smoothing parameter* $\lambda$ controls the amount of roughness.

- As $\lambda \to 0$, roughness matters less and less, and $x(t)$ fits the data better and better.
- As $\lambda \to \infty$, roughness matters more and more, and $x(t)$ becomes more and more "hyper–smooth."
- Our job is to find the right value where we trade enough bias off against sampling variance to minimize mean squared error.

# The roughness penalty matrix

- For the classic penalty,

$$\begin{aligned} \mathtt{PEN}_2(x) &= \int [D^2 \mathbf{c}' \phi(t)]^2 \, dt \\ &= \mathbf{c}' \int [D^2 \phi(t)][D^2 \phi'(t)] \, dt \, \mathbf{c} \\ &= \mathbf{c}' \mathbf{R} \mathbf{c} \end{aligned} \tag{1}$$

- The order $K$ *roughness penalty matrix* $\mathbf{R}$ is

$$\mathbf{R} = \int [D^2 \phi(t)][D^2 \phi'(t)] \, dt = \int (D^2 \phi)(D^2 \phi')$$

- substitute $L$ for $D^2$ for more general roughness penalties.

# The roughness penalized estimates for c and y

- $\mathbf{\Phi}$ is the $n$ by $K$ matrix of basis function values $\phi_k(t_j)$.
- The penalized least squares criterion becomes

$$\mathrm{PENSSE}(y|c) = (\mathbf{y} - \mathbf{\Phi c})'\mathbf{W}(\mathbf{y} - \mathbf{\Phi c}) + \lambda \mathbf{c}'\mathbf{R}\mathbf{c} \ .$$

- This is quadratic in $\mathbf{c}$, and is minimized by

$$\hat{\mathbf{x}} = (\mathbf{\Phi}'\mathbf{W}\mathbf{\Phi} + \lambda \mathbf{R})^{-1}\mathbf{\Phi}'\mathbf{W}\mathbf{y} \ .$$

## The smoothing matrix $\mathbf{S}_{\phi,\lambda}$

- The data-fitting vector $\hat{\mathbf{y}} = x(\mathbf{t})$ is

$$\hat{\mathbf{y}} = \mathbf{\Phi}(\mathbf{\Phi}'\mathbf{W}\mathbf{\Phi} + \lambda\mathbf{R})^{-1}\mathbf{\Phi}'\mathbf{W}\mathbf{y} \ ,$$

- Smoothing matrix

$$\mathbf{S}_{\phi,\lambda} = \mathbf{\Phi}(\mathbf{\Phi}'\mathbf{W}\mathbf{\Phi} + \lambda\mathbf{R})^{-1}\mathbf{\Phi}'\mathbf{W}$$

  maps the data into the fit, and has many useful applications.

# Equivalent degrees of freedom $df(\lambda)$

- It is useful to compare a fit using a roughness penalty to one using a fixed number of basis functions.
- A measure of the "degrees of freedom" in a roughness penalized fit is

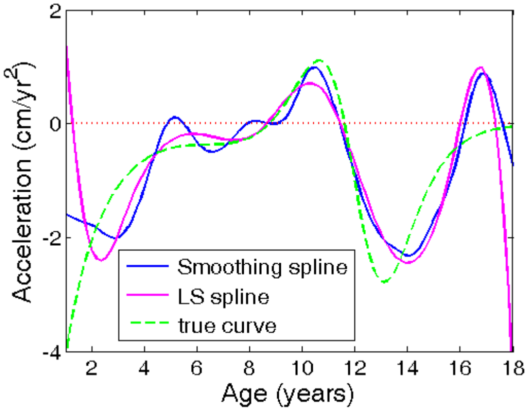
$$df(\lambda) = \text{trace}\, \mathbf{S}_{\phi,\lambda}$$

- This corresponds to the number of basis functions $K$ in an un–penalized fit.

# Outline

- The term “smoothing spline” has come to mean the following procedure:
  - Use natural or B-spline basis functions.
  - Place a knot at each data point $t_j$.
  - Use a penalty on $D^2x$.
- However, we find that
  - We can often achieve the same results by just using a number $K$ of basis functions that is “large” relative to the resolution of the data.
  - We certainly want to be able to play with alternative roughness penalties.
  - Other basis functions systems are also desirable.

# Two estimates of an acceleration curve.



# Outline

# Cross–validation for choosing the smoothing parameter $\lambda$

- In cross–validation,we
  - set aside a subset of data, the *validation sample*
  - call the balance of the data the *training sample*
  - fit the model to the training sample
  - assess fit to the validation sample
  - choose the $\lambda$ value that gives the best fit

- We can also, for a sequence of values of $\lambda$,
  - set aside each observation $(t_j, y_j)$ in turn
  - fit the data with the rest of the sample,
  - sum fits to the left out values to get a *cross–validated error sum of squares* $\mathrm{CV}(\lambda)$.
  - select the $\lambda$ value that minimizes $\mathrm{CV}(\lambda)$.

# Generalized cross–validation for choosing the smoothing parameter $\lambda$

- Cross-validation is time-consuming, and tends too often to under–smooth the data.
- The generalized cross-validation criterion is

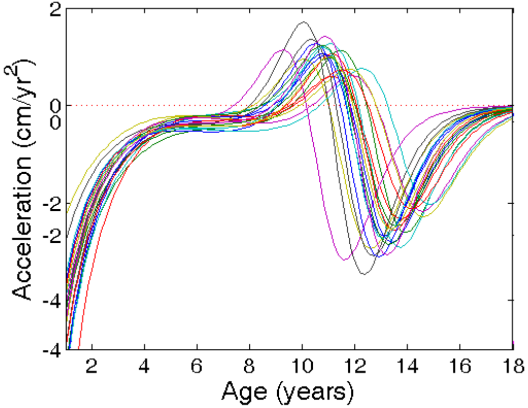
$$GCV(\lambda) = \left(\frac{n}{n - df(\lambda)}\right)\left(\frac{\mathrm{SSE}}{n - df(\lambda)}\right)$$

  where *df* is the equivalent degrees of freedom of the smoothing operator.
- The right factor is just the unbiassed estimate $s_e^2$ of residual variance familiar in regression analysis.
- The left factor further "discounts" this measure further to allow for the influence of optimizing with respect to $\lambda$.

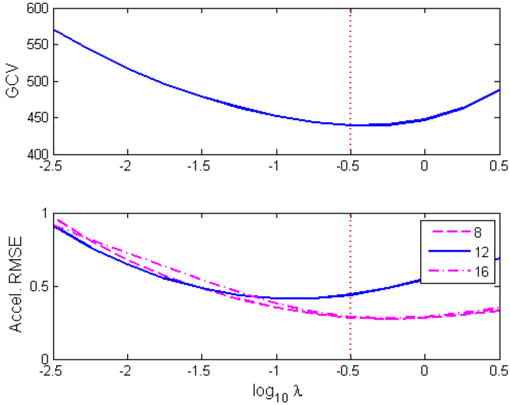
# Outline

- How does GCV work in a simulated data example?
- A parametric growth model by Pierre Jolicoeur at the Université de Montréal offers a nice test problem.
- We simulate 1000 samples, each observation being a random sample from realistic Jolicoeur models plus realistic error.
- We smooth using a range of values of $\lambda$, and note the value giving the best value of GCV.
- How well do we estimate the Jolicoeur acceleration curves?

# 20 Jolicoeur acceleration curves



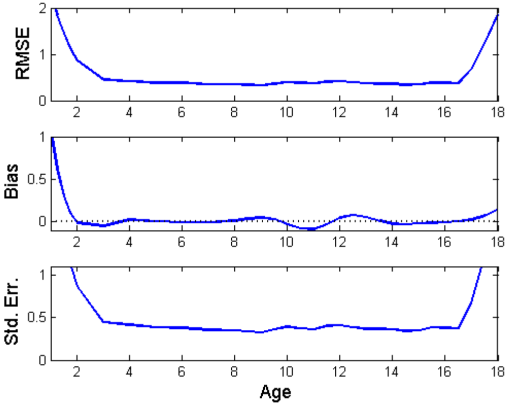
# GCV and Root-Mean-Squared-Error



# What we see

- In the top panel, GCV favors $\lambda = 0.1$.
- This is about right for optimal MSE for ages 8 and 16, but less smoothing would be better for age 12, in the middle of the pubertal growth spurt.
- One smoothing parameter value does not work best for all ages, but
- The value chosen by GCV certainly does a fine job.

# RMSE, Bias, and Standard Error



## What we see

- The performance of the spline smoothing estimate deteriorates badly at the extremes.
- The sharp curvature at the pubertal growth spurt also causes some problems.
- Except at the extremes and PGS, the bias is negligible.
- The standard error is about the same as RMSE.
- Would we do better at the extremes if the smooth respected monotonicity?

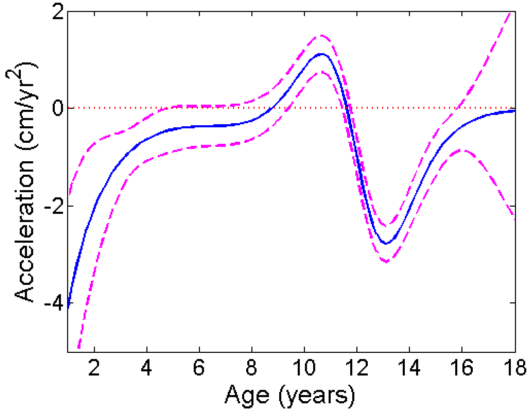
# Outline

- Because the mapping from data $\mathbf{y}$ to the coefficient vector $\mathbf{c}$ is linear, it is a simple matter to work out the standard error of any linear functional of a curve defined by $\mathbf{c}$.
- The variance of a quantity $\rho(x)$ associated with linear mapping $\mathbf{M}$ from $\hat{\mathbf{c}}$ to $\hat{\rho}(x)$ is

$$\texttt{Var}[\hat{\rho}(x)] = \mathbf{M}\mathbf{S}_{\phi,\lambda}\boldsymbol{\Sigma}_e\mathbf{S}_{\phi,\lambda}\mathbf{M}'$$

- Simple, that is, if we can get a good estimate of the variance-covariance matrix $\boldsymbol{\Sigma}_e$ of the residual vector.

# 95% point–wise confidence limits for growth acceleration



# Summary

- Roughness penalization, also called *regularization*, is a flexible and effective way to ensure that an estimated function is “smooth.”
- We can tailor the definition of “smooth” to our needs.
- The roughness penalty idea extends to any type of *functional parameter* that we want to estimate from the data.
- Roughness penalties are one of the main ways in which we exploit the smoothness that we assume in the process generating the data.

# Roughness and energy

- “Roughness” is like *energy* in physics
- Roughness requires energy to produce, and smoothness implies limited energy.
- Where we imagine that the amount of energy behind the data is limited, it is natural to assume smoothness.