

# **Spline Library in DRIP**

Lakshmi Krishnamurthy **v0.69**, 5 July 2014

### Overview

# Framework Symbology and Terminology

- 1. <u>Predictor Ordinates</u>: The segment independent/input values.
- 2. Response Values: The segment dependent/output values.
- 3.  $C^0$ ,  $C^1$ , and  $C^2$  Continuity:  $C^0$  refers to base function continuity.  $C^1$  refers to the continuity in the first derivative, and  $C^2$  refers to continuity in the second.
- 4. <u>Local Piece-wise Parameterized Splines</u>: Here the space formulation is in the local variate space that spans 0 to 1 within the given segment this is also referred to as piece-wise parameterization.
- 5. <u>Bias</u>: This is the first term in the Spline Objective Function essentially measures the exactness of fit.
- 6. <u>Variance</u>: This refers to the second and the subsequent terms in the Spline Objective Function essentially measures the curvature/roughness.

### Motivation

- 1. <u>Definition</u>: "**Spline** is a sufficiently smooth polynomial function that is piecewise-defined, and possesses a high degree of smoothness at the places where the polynomial pieces connect (which are known as *knots*)." [Spline (Wiki), Judd (1998), Chen (2009)]
- 2. <u>Drivers</u>:
  - a. Lower degree, gets rid of oscillation associated with the higher degrees [Runge's phenomenon (Wiki)]
  - b. Easy, accurate higher degree smoothness specification
- 3. <u>Basic Spline</u>: Covered in [Spline (Wiki), Bartels, Beatty, and Barsky (1987), Judd (1998), De Boor (2001), Fan and Yao (2005), Chen (2009), Katz (2011)].

4. <u>History</u>: Schoenberg (1946), Ferguson (1964), Epperson (1998).

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### **Calibration Framework**

### Introduction

- 1. <u>Definition</u>: Calibration is the process of inferring the latent state elastic properties from the specified inputs.
  - Calibration takes both the "mandatory" and the "desirable" classes of inputs to fully determine the elastic properties.
  - It makes sense to generate the calibration micro-Jacobians right at the calibration time.
- 2. <u>Classes of static fields</u>: Elastic and inelastic
  - Elastic Fields => The actual Latent State response variables that will be calibrated
    to. More generally, any latent state response field (Markov or not) that is inferred
    will be an elastic parameter.
  - Inelastic Fields => The Latent State predictor ordinate variables these are often explicitly "chosen" or "designed in".
    - Typically inelastic fields correspond to constitutive properties (e.g., dimensions of a solid body, instruments composing a curve, etc)
    - Inelastic properties may also impose invariant, calibration independent edge/boundary behavioral constraint on the elastic ones.
    - O Design Parameters (such as the  $C^k$  continuity parameters, roughness penalty derivative order, etc.) are inelastic parameters too, since they do not vary with changes to the calibrator input.
- 3. <u>Calibrator Creation</u>: On creation, objects acquire specific values for the constitutive inelastic fields. Volatile Latent State elastic fields may as yet be undefined.
  - Setting of the elastic fields => Latent State Elastic fields adjust or vary to the combination of inelastic fields + inputs (external), and are set by the calibration process.

- Change of inputs => Change of external calibration inputs changes only those
   Latent State elastic properties, not the inelastic ones.
- 4. <u>Calibration is Inference</u>: Since calibrated parameters are used for eventual prediction, calibration is essentially inference. Bayesian classification (an alternate, generalized calibration exercise) is inference too.
  - The terms calibration/inference/estimation are all sometimes used analogously.
     Where estimation estimates parameters, it performs inference. Where it predicts, it performs prediction.
  - Infer the Past vs. Predict the Future => You may infer the past quantification
    metric, as well as predict the future quantification metric/manifest measure.

    Therefore, in that sense, inference/prediction is relative only to the current time
    (and using earlier/later information).

#### 5. Calibration and entity-variate focus:

- De-convolving the instrument entity/measure combination is necessary for the extraction of the parameter set.
- Parameter calibration/parameterization etc: inherently involve parsimonization across the latent state predictor ordinate variate state space – this is where the models come in.
- 6. <u>Latent State Construction off of hard/soft signals</u>: Hard Signals are typically the truthness signals. Typically reduce to one calibration parameter per hard observation, and they include the following:
  - Actual observations => Weight independent true truthness signals
  - Weights => Potentially indicative of the truthness hard signal strength
     Soft signals are essentially signals extracted from inference schemes. Again, typically reduce to one calibration parameter per soft inference unit, and they include the following:
  - Smoothness signals => Continuity, first, second, and higher-order derivatives match one parameter per match.
  - Bayesian update metrics => Inferred using Bayesian methodologies such as maximum likelihood estimates, variance minimization, and error minimization techniques.

- 7. <u>Directionality Bias</u>: Directionality "bias" is inherent in calibration (e.g., left to right, ordered sequence set, etc:) this simplifies the solution space significantly, as it avoids simultaneous non-linearity. Therefore, the same directional bias also exists in the calibration nodal sequence.
- 8. Truthness/Smoothness vs. Information Propagation: In segment-by-segment calibration challenges associated with inferring a composite Latent State, if the inference is based purely off of the truthness measurements, the information directionality/propagation/flow is irrelevant. Notions such as  $C^k$  are important primarily owing to the smoothness axioms.
  - In general, it is trivial to get the segment elastics to respond to (via inference) purely truthness signals. However, if the existence of additional directionality/propagation/flow criteria is posited, those need to be accommodated too (splines constructed through the  $C^k$  criteria are one common way).
- 9. <u>Head Node Calibration</u>: Calibration of the head node is typically inherently different from the other nodes, because the inputs needed/used by it could be different. The other nodes use continuity/smoothness parameters, which the head node does not.
- 10. <u>Parameter Space Explosion</u>: Generally not a problem as long as it is segment-localized (in linear systems parlance, as long the Latent State matrix is tri-diagonal, or close to it), i.e., local information discovery does not affect far away nodes/segments.
  - Also maybe able to use optimization techniques to trim them.
- 11. <u>Live Calibrated Parameter Updating</u>: Use automatic differentiation to:
  - Estimate parametric Jacobians (or sub-coefficient micro-Jacobians) to the observed product measures.
  - Re-adjust the shifts using the hard-signal strength.
  - Update the parameters from the calculated shifts.
  - Re-construct the curve periodically (for increments, as opposed to a full re-build).
- 12. <u>Spline Segment Calibrator</u>: For a given segment, its calibration depends only on the segment local value set the other inputs come from the prior segments (except in the case of "left-most" segment, whose full set of inputs will have to be extraneously specified).

13. Block Diagonalization vs. Segment/Segment Calibration: Since segment-by-segment span calibration occurs through  $C^k$  transmission, it will effectively be block diagonal if it is a linear system, and hence computationally efficient (this also allows for explicitly setting segment level controls). In other words, although the local matrix is dense, the span-level matrix is still sparse,

#### 14. <u>Calibration Perspective of Supervised vs. Unsupervised:</u>

- Supervised Alternate View => Since supervised learning depends upon a
  training step, post supervised activity may be viewed as a post-inference systems,
  where the inference/calibration has already occurred during the training step (and
  parsimonization into the parameter step). So, post-training, the supervised
  machine is only used for prediction.
- Unsupervised Alternate View => Here, inference and prediction happen simultaneously.
- Hybrid Supervised/Unsupervised => Clearly no TRUE unsupervised are possible
   (as there are prior views on linearity, Markov nature, error process, basis spline
   representation choice, etc;). So unsupervised systems are typically mostly hybrid
   systems.

# **Latent State Specification**

- 1. <u>Latent State Specification</u>: The latent-state here refers to the state whose dependent response values we wish to calibrate/infer as a function of the predictor ordinate. For e.g., in fixed income finance, the Prevailing Interest Rate, the survival, the forward rate, FX spot/forward would each constitute a potentially separate latent state that needs to be inferred.
- 2. <u>Latent State Quantification Metric</u>: A given latent state may be described by one/more alternate, mutually exclusive quantification metric. Again, the discounting latent state may be quantified using a discount factor, zero rate etc:
- 3. <u>Manifest Measure</u>: The Latent State may be inferred using a variety of external experimental measurements each of which produces a convolved signal of the latent

state. Each such signal is referred to as a manifest metric. Again, the discounting latent state may be inferred from the cash instrument manifest metric, the swap rate manifest metric etc:

# **Spline Builder Setup**

### **Design Objectives behind Interpolating Splines**

- 1. Symbols and Definition:
  - Good overview of the desired characteristics is provided in Goodman (2002).
  - Data:  $\{x_i, y_i\} \in \mathbb{R}^2, i = 0, ..., N; x_0 < x_1 < ... < x_i < ... < x_N$
  - Interpolating function:  $f(x_i) = y_i$ ;  $f: [x_0, x_N] \rightarrow [R^2 \Rightarrow R]$
  - Optional Actual Function: g(x)
- 2. Monotonicity:  $f(x_i)$  increases with increase in  $y_i$  (and vice versa).
  - **Truly monotonic** means that the segment extrema match g(x) extrema.
  - **Co-monotone** =>  $f(x_i)$  increases with increase in  $y_i$  within the segment (and vice versa)
    - Strictly **co-monotone** implies that sub-segment **monotonicity** must also be met, so "**local monotonicity**" where **monotonicity** matches between  $f(x_i)$  and  $y_i$  at the segment level, is what is accepted here, there can be an inflection among segments in the immediate proximity of the data extrema.
  - At most, one extremum is allowed in  $\{x_i, x_{+1i}\}$ .
- 3. Convexity:  $f(x_i)$  should also be convex wherever  $y_i$  is convex (and vice versa).
  - At the segment level this becomes co-convex. As before strict co-convexity is
    often highly restrictive, so local convexity is preferred. The earlier established
    conditions should also satisfy convexity criteria.
  - Desirable to have at most one inflection in  $\{x_i, x_{+1i}\}$ .
- 4. Smoothness: Smoothness (also called shape-preserving) corresponds to the least curvature. Even  $C^0$  can be "smooth", and so is  $C^k$ .

- 5. <u>Locality</u>: **Locality** means that the dependence of f(x) is primarily only on  $f(x_i)$  and  $f(x_i)$ . This is advantageous to schemes that locally modify/insert the points.
- 6. Approximation Order: Approximation Order indicates the smallest polynomial degree by which f(x) departs from g(x) as the density of x increases. More formally, it is the m in  $||f g|| \approx O(h^m)$ , where  $h = \max\{x_{i+1} x_i : i = 0,...,N-1\}$ .
  - For spline segments where g(x) through g(x) are specified locally, the first degree of departure should the first degree of non-continuity infinitesimally for both polynomial and non-polynomial splines, i.e., it should be k+1 where the continuity criterion is  $C^k$ .

### 7. Other Desired Criteria:

- The interpolating proxy f(x) should be able to replicate the target g(x).
- Fairness loosely a measure of "pleasing to the eye".
- Possible f(x) invariance under variate scaling/reflection.
- Controlled derivative behavior => Small changes in x produce small changes in f(x).
- 8. <u>Assessment of Monotonicity and Convexity</u>: An individual segment can be assessed to be monotone/convex etc:, but from the data PoV, peaks, valleys, and inflection occur only at the knots. These can be assessed only at the span level.

### **Base Formulation**

- 1. Base Mathematical formulation:
  - $y(x) = \sum_{i=0}^{n-1} a_i f_i(x)$ , therefore  $\frac{d^r y(x)}{dx^r} = \sum_{i=0}^{n-1} a_i \frac{d^r f_i(x)}{dx^r}$ .
  - From known nodes  $\{x_0, y_0\}$  and  $\{x_1, y_1\}$ , we can draw the 2 linear equations for  $a_i$ :

$$\circ y(0) = \sum_{i=0}^{n-1} a_i f_i(0)$$

$$\circ y(1) = \sum_{i=0}^{n-1} a_i f_i(1)$$

• From known nodal derivatives  $\{x_0, y_k(x_0)\}_{k=1}^r$ , where  $y_k(x_0) = \left[\frac{d^k y}{dx^k}\right]_{x_0}$ , we can draw the following r linear equations for  $a_i$ :

$$\circ y_k(0) = \sum_{i=0}^{n-1} a_i \left[ \frac{d^k f_i(x)}{dx^k} \right]_{x=x_0} \text{ where } k \Rightarrow 1, \dots, r$$

2. Linear of Segment Coefficients to the Response Values ( $y_i$ ): In all the spline

formulations, the Jacobian  $\frac{\partial C_j}{\partial y_i}$  is constant (i.e., independent of the response values or their nodal derivative inputs).

- 3. Span Boundary Specification:
  - "Natural" Spline Energy minimization problem Second Derivative is Zero at either of the extreme nodes.
  - "Financial" Spline Second Derivative at the left extreme is zero, but first derivative at the right extreme is zero.
  - Clamped Boundary Conditions:  $\left[\frac{\partial f}{\partial x}\right]_{x=x_0} = \alpha$ , and  $\left[\frac{\partial f}{\partial x}\right]_{x=x_N} = \beta$ .
  - Not-A-Knot Boundary Conditions:  $\left[\frac{\partial^3 f}{\partial x^3}\right]_{x=x_0} = \left[\frac{\partial^3 f}{\partial x^3}\right]_{x=x_1}$  and

$$\left[\frac{\partial^3 f}{\partial x^3}\right]_{x=x_{N-1}} = \left[\frac{\partial^3 f}{\partial x^3}\right]_{x=x_N}.$$

- 4. <u>Discrete Segment Mesh vs. Inserted Knots</u>: Inserting knot point is similar to discretizing the segment into multiple grids, with one key difference:
  - Discretization uses the same single spline across all the grid units of the segment.
  - Inserted knots introduce additional splines on between each knot pair.
- 5. <u>Segment Inelastics</u>: These are effectively the same as shape controller, i.e., the following are the shape controlling inelastic parameter set:
  - Tension  $\sigma$

- Number of basis *n*
- Continuity  $C^k$
- Optimizing derivative set order *m*

# **B-Splines**

### Introduction

- Motivation: As postulated by De Boor et. al. (see De Boor (2001)), B Splines have a
  geometric interpolant context thereby with the correspondingly strong
  CADG/curve/surface construction focus. Smoothening occurs as a natural part of this.
  - The B Spline generation scheme has a recurrence-based iterative polynomial generator that admits coinciding control points facilitate and surface construction, with shape-preserving interpolation control thrown in.
- 2.  $\underline{k^{th} \text{ Order B-Spline Interpolant}}$ : Higher order B-Splines are defined by the recurrence  $B_{i,k} = \varepsilon_{i,k} B_{i,k-1} + (1 \varepsilon_{i+1,k}) B_{i+1,k-1}$  where  $\varepsilon_{i,k} = \frac{t t_i}{t_{i+k-1} t_i}$  and  $B_{i1}(t) = X_i(t) = 1$  if  $t_i < t < t_{i+1}$ , and  $B_{i1}(t) = X_i(t) = 0$  otherwise.
  - Coinciding knots  $\Rightarrow t_i = t_{i+1} \rightarrow B_{i1} = 0$ .
- 3. Recursive Interpolant Scheme: B Spline formulation is recursively interpolant, i.e., the order k spline is interpolant over the order k-1 splines on nodes i and i+1 this formulation automatically ensures  $C^{k-2}$  nodal continuity.
  - As shown in Figure 4, the left interpolator stretch [i, i+k-1] contains the interpolator pivot at  $t_i$ , and the right interpolator stretch [i+1, i+k] contains the interpolator pivot at  $t_{i+1}$ .
  - $B_{p,q}$  spans all the segments between the nodes [p..q].
  - Further, the formulation symmetry between the left pivot at  $B_{i,k-1}$  and the right pivot at  $B_{i+1,k-1}$  retains the interpolation symmetry among other things, it is responsible for ensuring the  $C^{k-2}$  symmetry.
- 4. <u>B-Spline Order Relationships</u>: Assuming no coincident knots, the following statements are all EQUIVALENT/TRUE:
  - n+1 knot points.

- n<sup>th</sup> order B Spline.
- Polynomial of degree n-1.
- Continuity criterion  $C^{n-2}$ .
- 5. Expository Formulation:

$$\bullet \quad B_{i,k} = \sum_{j=0}^{k} \alpha_{ij} X_{i+j}$$

$$\bullet \quad \alpha_{i0} = \varepsilon_{i,k-1}...\varepsilon_{i0} = \prod_{j=k-1}^{0} \varepsilon_{i,j} \text{ where } \varepsilon_{i,j} = \frac{t - t_{i+j-1}}{t_{i+j} - t_{i+j-1}}$$

$$\bullet \quad \alpha_{ik} = \prod_{l=1}^{k} \left[ 1 - \varepsilon_{i+l-1} \right] \text{ where } \varepsilon_{i+l-1} = \frac{t - t_{i+l-1}}{t_{i+l} - t_{i+l-1}}$$

6. Spline Coefficient Partition of Unity: Using the earlier formulation  $B_{i,k} = \sum_{j=0}^{k} \alpha_{ij} X_{i+j}$ ,

it is easy to show that  $\sum_{j=0}^{k} \alpha_{ij} = 1$ . This simply follows from the recursive nodal interpolation property.

- 7. <u>Smoothness Multiplicity Order Linker</u>: # smoothness conditions at knot + the multiplicity at the knot = B-Spline Order.
- 8. <u>Starting Node de-biasing</u>: Left node is always weighted by  $\varepsilon_{i,k}$  in the interpolation scheme, but the left node asymmetry is maintained because the denominator in

$$\varepsilon_{i,j} = \frac{t-t_{i+j-1}}{t_{i+j}-t_{i+j-1}}, \text{ i.e., } t_{i+j}-t_{i+j-1} \text{ increases in length.}$$

- 9. Other Single B-Spline Properties:
  - $B_{ik}$  is a piece-wise polynomial of degree < k (k-1 if the knots are distinct, lesser if the some of the knots coincide).
  - $B_{ik}$  is zero outside of  $[t_i, t_{i+k})$ .
  - $B_{ik}$  is positive in the open interval  $[t_i,...,t_{i+k}]$ .
- 10. Formulation off of Starting Node and Starting Order: Given the starting node i and the starting order k, the contribution to the node i + m (i.e., m nodes after the start)

and the order (i.e., n nodes after start) can be "series" ed as

$$B_{i+m,k-n} = \mathbf{N}\big(i+m,k-n+1 \longrightarrow k-n\big)B_{i+m,k-n} + \mathbf{B}\big(i+m-1 \longrightarrow i+m,k-n\big)B_{i+m+1,k-n}$$

• Nodal B-Spline Recursion Stepper:

$$N(i+m,k-n+1 \to k-n) = \wp(i+m \to i+m,k-n+1 \to k-n)$$

$$= \left[\frac{t-t_{i+m}}{t_{i+m+k-n+1}-t_{i+m}}\right] \left[\frac{t_{i+m+k-n}-t}{t_{i+m+k-n}-t_{i+m+1}}\right]$$

• Spline Order B Spline Recursion Stepper:

$$B(i+m-1 \to i+m, k-n) = \wp(i+m-1 \to i+m, k-n \to k-n)$$

$$= \left[\frac{t-t_{i+m}}{t_{i+m+k-n+1}-t_{i+m}}\right] \left[\frac{t-t_{i+m+1}}{t_{i+m+k-n}-t_{i+m+1}}\right]$$

- 11. <u>Cardinal B-Spline Knot Sequence</u>: Knot sequence  $Z \Rightarrow$  Uniformly spaced knots, simplifying the interpolant/recursive analysis significantly  $Z \Rightarrow \{...,-2,-1,0,1,2,...\}$ .
  - Also all Cardinal B-Splines of a given order k are translates of each other.
  - Cardinal B-Spline Order 2:

Range	$B_{i,2}$	$B_{i+1,2}$
0 ≤ <i>t</i> < 1	t	0
$1 \le t < 2$	2-t	t-1
$2 \le t < 3$	0	3-t

• Cardinal B-Spline Order 3:  $B_{i,3} = \frac{t}{2}B_{i,2} + \frac{3-t}{2}B_{i+1,2}$ 

Range	$B_{i,3}$	$rac{\partial B_{i,3}}{\partial t}$
0 ≤ <i>t</i> < 1	$\frac{1}{2}t^2$	t
1 ≤ <i>t</i> < 2	$\frac{1}{2}\left(-2t^2+6t-3\right)$	-2t-3
2 ≤ <i>t</i> < 3	$\frac{1}{2}(t-3)^2$	t-3

### 12. Non-coinciding B Spline Segment Relations:

• 
$$B_{i,1} = X_i = 1 \text{ if } t_i \le t < t_{i+1}$$

• 
$$B_{i,1} = X_i = 0$$
 outside

$$\bullet \quad B_{i,2} = \left[ \frac{t - t_i}{t_{i+1} - t_i} \right] X_0 + \left[ \frac{t_{i+2} - t}{t_{i+2} - t_{i+1}} \right] X_1$$

$$\bullet \quad B_{i+1,2} = \left[\frac{t - t_{i+1}}{t_{i+2} - t_{i+1}}\right] X_1 + \left[\frac{t_{i+3} - t}{t_{i+3} - t_{i+2}}\right] X_2$$

$$\bullet \quad B_{i,3} = \left[\frac{t - t_i}{t_{i+2} - t_i}\right] B_{i,2} + \left[\frac{t_{i+3} - t}{t_{i+3} - t_{i+i}}\right] B_{i+1,2}$$

Range	$B_{i,2}$	$B_{i+1,2}$	$B_{i,3}$
$t_i \le t < t_{i+1}$	$\frac{t - t_i}{t_{i+1} - t_i}$	0	$\frac{t-t_i}{t_{i+2}-t_i}\frac{t-t_i}{t_{i+1}-t_i}$
$t_{i+1} \le t < t_{i+2}$	$\frac{t_{i+2}-t}{t_{i+2}-t_i}$	$\frac{t - t_{i+1}}{t_{i+2} - t_{i+1}}$	$\frac{t-t_i}{t_{i+2}-t_i}\frac{t_{i+2}-t}{t_{i+2}-t_{i+1}} + \frac{t_{i+3}-t}{t_{i+3}-t_{i+1}}\frac{t-t_{i+1}}{t_{i+2}-t_{i+1}}$
$t_{i+2} \le t < t_{i+3}$	0	$\frac{t_{i+3} - t}{t_{i+3} - t_{i+1}}$	$\frac{t_{i+3} - t}{t_{i+3} - t_i} \frac{t_{i+2} - t}{t_{i+2} - t_{i+1}}$

13. <u>Bernstein B-Spline Knot Sequence</u>: Knot sequence  $\Xi \Rightarrow \{0,...,0,1,...,1\}$  -  $\{0,...,0\}$  occurs  $\mu$  times, and  $\{1,...,1\}$  occurs  $\nu$  times.

• 
$$B[\mu, \nu, t] = \frac{(\mu + \nu)!}{\mu! \nu!} (1 - t)^{\mu} t^{\nu} \text{ for } 0 \le t < 1.$$

- $B[\mu, \nu, t]$  has  $\nu 1$  derivatives at t = 0, and  $\mu 1$  derivatives at t = 1 this is also referred to as  $\nu$  smoothness conditions at t = 0, and  $\mu$  smoothness conditions at t = 1.
- 14. <u>B-Spline vs. Spline</u>: B-Spline is just a single basis polynomial that is valid across a set of knots. "**Spline**" is a linear combination of such basis B Splines i.e., the set of all the  $B_{ik}$  's.
- 15. Spline Definition:  $S_{k,t} = \sum_{i} B_{ik} a_i$  where  $a_i \in R^1$ .  $a_i$ 's are the coefficients or nodal points  $\{x_i, a_i\}$  that can be interpolated.

### **B Spline Derivatives**

1. B-Spline Derivative Formulation:

$$\bullet \quad \frac{\partial^r B_{i,k}}{\partial t^r} = \left[ \frac{r}{t_{i+k-1} - t_i} \right] \frac{\partial^{r-1} B_{i,k-1}}{\partial t^{r-1}} + \left[ \frac{t - t_i}{t_{i+k-1} - t_i} \right] \frac{\partial^r B_{i,k-1}}{\partial t^r} - \left[ \frac{r}{t_{i+k} - t_{i+1}} \right] \frac{\partial^{r-1} B_{i+1,k-1}}{\partial t^{r-1}} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} - \left[ \frac{r}{t_{i+k} - t_{i+1}} \right] \frac{\partial^{r-1} B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t_{i+1}} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} - t} \right] \frac{\partial^r B_{i+1,k-1}}{\partial t^r} + \left[ \frac{t_{i+k} - t}{t_{i+k} -$$

2. <u>B Spline Order 3 Nodal Slopes</u>: The slopes match across the left and the right segment, as shown below, thereby making  $B_{3,i}$   $C^1$  continuous.

Range	Left Slope	pe Right Slope	
$t_i$	-	0	
$t_{i+1}$	$\frac{t_{i+1}-t}{t_{i+2}-t_i}$	$\frac{t_{i+1}-t}{t_{i+2}-t_i}$	
$t_{i+2}$	$\frac{t_{i+3} - t_i}{t_{i+2} - t_{i+1}}$	$\frac{t_{i+3} - t_i}{t_{i+2} - t_{i+1}}$	
$t_{i+3}$	0	-	

3. <u>B Spline Continuity Condition</u>: From the B Spline derivative formulation it is clear that if both  $B_{i,k-1}$  and  $B_{i+1,k-1}$  are  $C^{k-3}$  continuous, then  $B_{i,k}$  will be  $C^{k-2}$  continuous. Given that B Spline order 3 is  $C^1$  continuous, by induction,  $B_{i,k}$  is  $C^{k-2}$  continuous.

# **Polynomial Spline Basis Function**

### **Plain Polynomial Spline Basis Function**

- 1. Most direct polynomial spline fit is the Lagrange polynomial that passes through the sequence of given points.
- Young (1971) was one of first to apply shape-preserving polynomial using diminished Lagrange Polynomials (Lagrange Polynomials (Wiki)), showing that comonotone interpolant with an upper bound on the polynomial degree exists (Raymon (1981)).
- 3. <u>Knot Insertion and Control Techniques</u>: Careful knot insertion can produce:
  - Convexity Preserving Schemes on C<sup>2</sup> cubic (de Boor (2001)).
  - Co-monotone, co-convex schemes on C<sup>1</sup> quadratic (McAllister and Roulier (1981a), McAllister and Roulier (1981b), Schumaker (1983)).
  - Co-monotone on C<sup>1</sup> cubic (Butland (1980), Fritsch and Butland (1984), Fritsch and Carlson (1980), Utreras and Celis (1983)).
  - Co-monotone and co-convex on C<sup>1</sup> cubic (Costantini and Morandi (1984)).
  - C<sup>2</sup> co-monotone and co-convex by using cubic in any interval where there is an inflection, and linear/quadratic rational elsewhere (Schaback (1973), Schaback (1988)).

# **Bernstein Polynomial Basis Function**

- 1. Bernstein Polynomial of degree n, and term  $\underline{v}$ :  $b_{v,n}(x) = {}^{n}C_{v}x^{v}(1-x)^{n-v}$  where v = 0,...,n.
  - Bernstein Polynomial Convenience Re-cast #1:  $b_{\nu,n}(x) = n! \frac{x^{\nu}}{\nu!} \frac{(1-x)^{n-\nu}}{(n-\nu)!}$ .

- Bernstein Polynomial Convenience Re-cast #2:  $P_{b,c}(x) = (b+c)!F(x,b)F(1-x,c)$  where  $F(x,b) = \frac{x^b}{b!}$ .
- 2. <u>Derivative of the Bernstein Polynomial</u>:  $\frac{d^r b_{v,n}(x)}{dx^r} = n \left[ \frac{d^{r-1} b_{v-1,n}(x)}{dx^{r-1}} \frac{d^{r-1} b_{v-1,n-1}(x)}{dx^{r-1}} \right].$ 
  - Bernstein Polynomial Re-cast #2 Derivative:

$$\frac{\partial P_{b,c}(x)}{\partial x} = (b+c)! \left[ \frac{\partial F(x,b)}{\partial x} F(1-x,c) + F(x,b) \frac{\partial F(1-x,c)}{\partial x} \right].$$

- 3. <u>Bernstein Recurrence</u>:  $b_{\nu,n}(x) = (1-x)b_{\nu,n-1}(x) + xb_{\nu-1,n-1}(x)$ .
- 4. Reduction of B-Splines to Bernstein's Polynomial: From the recurrence relation, it is clear that this is exactly the same recurrence as that for B-splines, except that it happens over repeating knots at x = 0 and x = 1.
  - Further,  $b_{0,i} = 1$  for  $0 \le x < 1$ , and  $b_{0,i} = 0$  otherwise.

# **Local Spline Stretches**

### **Local Interpolating/Smoothing Spline Stretches**

- 1. <u>Hermite Cubic Splines</u>: The "local information" here takes the form of user specified left/right slopes + calibration points.
  - 2 User Specified local slopes + 2 points => 4 sets of equations. Solve for the coefficients.
  - C¹ continuity is maintained, and C² continuity is not.
  - Segment control is completely local. Both the head and non-head calibration are identical/analogous for this reason.
- 2. <u>C¹ Hermite Formal Definition</u>: For C¹, the Hermite polynomial of degree 2n+1 is given as  $H_{2n+1}(x) = \sum_{j=0}^{n} \{f_j H_{n,j}(x) + f_j \dot{H}_{n,j}(x)\}$ , where  $H_{n,j}(x)$  and  $\hat{H}_{n,j}(x)$  are expressed in terms of the j<sup>th</sup> Lagrange coefficient of degree n,  $L_{n,j}(x)$  as
  - $H_{n,j}(x) = [1 2(x x_j)L_{n,j}'(x)]L_{n,j}^2(x)$
  - $\bullet \quad \hat{H}_{n,i}(x) = \left[x x_i\right] L_{n,i}^{2}(x)$
- 3. <u>Catmull-Rom Cubic Splines (Catmull and Rom (1974))</u>: Instead of explicitly specifying the left/right segment slopes, they are inferred from the "averages" of the prior and the subsequent points, i.e.,  $\vec{\tau}_i = \frac{1}{2} \left[ \vec{p}_{i+1} \vec{p}_{i-1} \right]$ , and  $\vec{\tau}_{i+1} = \frac{1}{2} \left[ \vec{p}_{i+2} \vec{p}_i \right]$ . Here  $\vec{\tau}_i$  refers to the slope vector, and  $\vec{p}_i$  to the point vector.
  - Again, C<sup>1</sup> continuity is maintained, and C<sup>2</sup> continuity is not.
  - Segment control is not completely local, but still local enough it only depends on the neighborhood of 3 points.

- 4. <u>Cardinal Cubic Splines</u>: This is a generalization of the Catmull-Rom spline with a tightener coefficient  $\sigma$ , i.e.,  $\overrightarrow{\tau}_i = \frac{1}{2} (1 \sigma) \left[ \overrightarrow{p}_{i+1} \overrightarrow{p}_{i-1} \right]$ , and  $\overrightarrow{\tau}_{i+1} = \frac{1}{2} (1 \sigma) \left[ \overrightarrow{p}_{i+2} \overrightarrow{p}_i \right]$ .  $\sigma > 0$  corresponds to tightening, and  $\sigma < 0$  corresponds to loosening.
  - Again, C<sup>1</sup> continuity is maintained, and C<sup>2</sup> continuity is not.
  - Segment control is "local" in the Catmull-Rom sense it only depends on the neighborhood of 3 points.
- Catmull-Rom/Cardinal Splines as Interpolation Splines: As interpolating splines, both Catmull-Rom and Cardinal are primarily useful in heuristic knot-insertions – Catmull-Rom as linear in the gaps, and Cardinal as tense linear gap knots.
  - The local knot point insertion may be generalized as follows: The targeted knot insertions follow the formulation paradigm  $f(x_{KNOT}) = f(x_i : i \forall \aleph)$ , where  $\aleph$  is the set of the neighborhood points. Similar formulation (with potentially different function forms, of course) may be used for each of the  $C^k$  derivatives. Catmull-Rom and cardinal use 1D, strictly neighboring adjacencies, as well as tense linear averaging.
- 6. <u>C¹ Hermite-Bessel Splines</u>: These splines use 4 basis functions per segment, therefore they are cubic polynomial, but  $C^1$ . The first are set at each node  $x_i$  as the first derivative of the quadratic that passes through  $x_{i-1}$ ,  $x_i$ , and  $x_{i+1}$  (the edges are handled slightly differently, as shown below). Specifically:

• 
$$b_0 = \frac{1}{x_2 - x_0} \left[ \frac{(x_2 + x_1 - 2x_0)(y_1 - y_0)}{(x_1 - x_0)} - \frac{(x_1 - x_0)(y_2 - y_1)}{(x_2 - x_1)} \right]$$

• 
$$b_n = \frac{1}{x_n - x_{n-2}} \left[ \frac{(x_n - x_{n-1})(y_{n-1} - y_{n-2})}{(x_{n-1} - x_{n-2})} - \frac{(2x_n - x_{n-1} - x_{n-2})(y_n - y_{n-1})}{(x_n - x_{n-1})} \right]$$

• 
$$b_i = \frac{1}{x_{i+1} - x_{i-1}} \left[ \frac{(x_{i+1} - x_i)(y_i - y_{i-1})}{(x_i - x_{i-1})} + \frac{(x_i - x_{i-1})(y_{i+1} - y_i)}{(x_{i+1} - x_i)} \right]$$
 for  $1 \le i < n - 1$ 

- 7. Hyman's Monotone Preserving Cubic Spline:
  - Hyman (1983) applies the stringent conditions to preserve monotonicity by applying the de Boor-Schwarz criterion.

- Define  $m_i = \frac{y_{i+1} y_i}{x_{i+1} x_i}$ . If locally monotone (i.e.,  $m_{i-1}m_i \ge 0$ ), then set  $b_i = \frac{3m_{i-1}m_i}{\max[m_{i-1},m_i] + 2\min[m_{i-1},m_i]}$ . If non-monotone (i.e.,  $m_{i-1}m_i < 0$ ), then set  $b_i \ge 0$ .
- Put another way (Iwashita (2013)): For cubic polynomial splines, the first derivative should be in the range  $\frac{-3\tau_i f_i}{h_i} \le \tau_i f_i' \le \frac{3\tau_i f_i}{h_{i-1}}$  where  $\tau_i \Longrightarrow sign(f_i)$ .
- Adjustment for Spurious Extrema => To ensure that no spurious extrema is introduced in the interpolant,  $b_{i,Adj} = \min[\max(0,b_i),3*\min(m_{i-1},m_i)]$  if  $y_{i+1} > y_i$ , and  $b_{i,Adj} = \max[\min(0,b_i),3*\max(m_{i-1},m_i)]$  if  $y_{i+1} < y_i$ .
- 8. <u>Hyman89 Extension to Hyman83</u>: Doherty, Edelman, and Hyman (1989) relax the Hyman83 stringency posited for monotonicity preservation. Define the following:

• 
$$\mu_{i,-1} = \frac{m_{i-1}[2(t_i - t_{i-1}) + t_{i-1} - t_{i-2}] + m_{i-2}(t_i - t_{i-1})}{t_i - t_{i-2}}$$

• 
$$\mu_{i,0} = \frac{m_{i-1}(t_{i+1} - t_i) + m_i(t_i - t_{i-1})}{t_{i+1} - t_{i-1}}$$

• 
$$\mu_{i,1} = \frac{m_i [2(t_{i+1} - t_i) + t_{i+2} - t_{i+1}] - m_{i+1}(t_{i+1} - t_i)}{t_{i+2} - t_i}$$

• 
$$M_i = 3 * \min[|m_{i-1}|, |m_i|, |\mu_{i,0}|, |\mu_{i,1}|]$$

- If i > 2,  $\mu_{i,-1}$ ,  $\mu_{i,0}$ ,  $(m_{i-1} m_{i-2})$ , and  $(m_i m_{i-1})$  all have the same sign, then  $M_i = \max \left[ M_i, 1.5 * \min \left( |\mu_{i,0}|, |\mu_{i,-1}| \right) \right].$
- If i > n-1,  $-\mu_{i,0}$ ,  $-\mu_{i,1}$ ,  $(m_i m_{i-1})$ , and  $(m_{i+1} m_i)$  all have the same sign, then  $M_i = \max \left[ M_i, 1.5 * \min \left( |\mu_{i,0}|, |\mu_{i,-1}| \right) \right]$ .
- Finally, set  $s_i = sign(s_i) * min[M_i, |s_i|]$  if  $sign(s_i) = sign(\mu_{i,0})$ , and  $s_i = 0$  otherwise.
- 9. Hyman's Monotone Preserving Quintic Spline:
  - For quintic polynomial splines, the first derivative should be in the range  $\frac{-5\tau_i f_i}{h} \le \tau_i f_i' \le \frac{5\tau_i f_i}{h} \text{ where } \tau_i \Longrightarrow sign(f_i).$

• The constraint on the second derivative is:

$$\tau_i f_i \leq \tau_i \max \left[ 8 \frac{f_i}{h_{i-1}} - 20 \frac{f_i}{h_{i-1}^2}, -8 \frac{f_i}{h_i} - 20 \frac{f_i}{h_i^2} \right].$$

- Monotonicity Preserving Quintic Spline => Enhancement of the criterion established by de Boor and Schwartz (1977) (Hyman (1983), Doherty, Edelman, and Hyman (1989)).
  - o Set  $\sigma_i = sign(f_i)$  if  $s_{i-1}s_i < 0$ , and  $\sigma_i = 0$  otherwise. Then
  - o If  $\sigma_i \ge 0$ , then  $f_i' = \min[\max(0, f_i'), 5\min(|s_{i-1}|, |s_i|)]$ , AND:
  - o If  $\sigma_i \le 0$ , then  $f_i' = \max[\min(0, f_i'), -5\min(|s_{i-1}|, |s_i|)]$ .
- Second Derivative Tests for Monotonicity Preserving Quintic Spline =>
  - o Define the following constants:

$$a = \max \left[ 0, \frac{f_i'}{s_{i-1}} \right].$$

$$b = \max \left[ 0, \frac{f_{i+1}}{s_i} \right].$$

- $d_+ = f_i$  if  $f_i$ '  $s_i > 0$ , and  $d_+ = 0$  otherwise.
- $d_{-} = f_{i}'$  if  $f_{i}' s_{i-1} > 0$ , and  $d_{-} = 0$  otherwise.
- O Define Ranges A and B as:

$$A = \left[ \frac{-7.9d_{+} - 0.26d_{+}b}{h_{i}}, \frac{(20 - 2b)s_{i} - 8d_{+} - 0.48d_{+}a}{h_{i}} \right], \text{ AND}$$

$$B = \left\lceil \frac{(2a - 20)s_{i-1} + 8d_{-} + 0.48d_{-}a}{h_{i-1}}, \frac{7.9d_{-} + 0.26d_{-}b}{h_{i-1}} \right\rceil.$$

If A and B overlap, then  $f_i$  should lie in their common range. If they do not overlap,

i.e., 
$$A \cap B \Rightarrow \Phi$$
, reset  $f_i$ ' as  $f_i$ ' =  $\frac{\frac{(20-2b)s_i}{h_i} + \frac{(20-2a)s_{i-1}}{h_{i-1}}}{\frac{8+0.48b}{h_i} + \frac{8+0.48a}{h_{i-1}}}$ . Setting this  $f_i$ ' ensures

that A and B overlap, so the other tests aspects may now continue.

10. Harmonic Splines: Introduced by Fritsch and Butland (1984) as:

• 
$$\frac{1}{s_i} = \frac{t_i - t_{i-1} + 2[t_{i+1} - t_i]}{3[t_{i+1} - t_{i-1}]} \frac{1}{m_{i-1}} + \frac{2[t_i - t_{i-1}] + t_{i+1} - t_i}{3[t_{i+1} - t_{i-1}]} \frac{1}{m_i}$$
 if  $m_{i-1}m_i > 0$ ,  $s_i = 0$  if

 $m_{i-1}m_i \leq 0$ . Boundary Conditions are:

• 
$$s_0 = \frac{t_2 - t_1 + 2[t_1 - t_0]}{t_2 - t_0} m_0 - \frac{t_1 - t_0}{t_2 - t_0} m_1$$

$$\bullet \qquad s_0 = -\frac{t_n - t_{n-1}}{t_n - t_{n-2}} m_{n-2} + \frac{t_{n-1} - t_{n-2} + 2[t_n - t_{n-1}]}{t_n - t_{n-2}} m_{n-1}$$

• Harmonic Spline Monotonicity Filter =>

$$\circ$$
  $s_0 = 3 * m_0 \text{ if } s_0 m_0 > 0 \text{ AND } m_0 m_1 \le 0 \text{ AND } |s_0| < |3 * m_0|$ 

$$\circ$$
  $s_0 = s_0 \text{ if } s_0 m_0 > 0$ 

$$\circ s_0 = 0 \text{ if } s_0 m_0 \le 0$$

o 
$$s_n = 3 * m_{n-1}$$
 if  $s_n m_{n-1} > 0$  AND  $m_{n-1} m_{n-2} \le 0$  AND  $|s_n| < |3 * m_{n-1}|$ 

$$\circ s_n = s_n \text{ if } s_n m_{n-1} > 0$$

$$\circ \quad s_n = 0 \text{ if } s_n m_{n-1} \le 0$$

• Continuous Limiters => For harmonic splines, as the predictor ordinate widths

become identical 
$$(t_i - t_{i-1} = t_{i+1} - t_i)$$
, setting  $r = \frac{m_i}{m_{i-1}}$ , we get  $s_i = m_i \frac{r + |r|}{1 + |r|}$ . This is the

Van Leer limit (Van Leer (1974)). Huynh (1993) reviews several such limiters.

 Shortcoming of these Limiters => Since they rely on min/max/modulus functions, by definition they are not smooth close to transition edge. This is rectified by Le Floc'h (2013), who defines a new limiter based on rational functions:

$$s_i = \frac{3m_i m_{i-1} (m_i + m_{i-1})}{m_i^2 + 4m_i m_{i-1} + m_i^2}$$
 for  $m_i m_{i-1} > 0$ , and  $s_i = 0$  otherwise. This produces a stable

 $C^1$  interpolator.

#### 11. Akima Cubic Interpolator (Akima (1970)):

• Expand the Predictor Ordinates => Add 2 predictor ordinates each at the left and the right boundaries using  $(x_{-2}, x_{-1}, x_{N+1}, x_{N+2})$ :

$$o \quad x_{N+2} - x_N = x_{N+1} - x_{N-1} = x_N - x_{N-2}$$

• Expand the Response Values => Add 2 response values each at the left and the right boundaries using  $(y_{-2}, y_{-1}, y_{N+1}, y_{N+2})$  using:

$$\circ \quad \frac{y_{N+2} - y_{N+1}}{x_{N+2} - x_{N+1}} - \frac{y_{N+1} - y_{N}}{x_{N+1} - x_{N}} = \frac{y_{N+1} - y_{N}}{x_{N+1} - x_{N}} - \frac{y_{N} - y_{N-1}}{x_{N} - x_{N-1}} = \frac{y_{N} - y_{N-1}}{x_{N} - x_{N-1}} - \frac{y_{N-1} - y_{N-2}}{x_{N-1} - x_{N-2}}$$

$$\circ \quad \frac{y_{-2} - y_{-1}}{x_{-2} - x_{-1}} - \frac{y_{-1} - y_0}{x_{-1} - x_0} = \frac{y_{-1} - y_0}{x_{-1} - x_0} - \frac{y_0 - y_1}{x_0 - x_1} = \frac{y_0 - y_1}{x_0 - x_1} - \frac{y_1 - y_2}{x_1 - x_2}$$

• Final  $C^1$  Slope => Compute the final Akima  $C^1$  slopes using:

o If 
$$s_{i+1} \neq s_i$$
 OR  $s_{i-1} \neq s_{i-2}$ , then  $f_i' = \frac{|s_{i+1} - s_i| |s_{i-1} + |s_{i-1} - s_{i-2}| |s_i|}{|s_{i+1} - s_i| + |s_{i-1} - s_{i-2}|}$ .

Otherwise 
$$f_i' = \frac{s_i + s_{i-1}}{2}$$
.

12. Kruger's Constrained Cubic Interpolant (Kruger (2002)):

- $f_i = 0$  if  $s_i s_{i-1} > 0$ .
- $f_i' = \frac{2}{\frac{1}{s_i} + \frac{1}{s_{i-1}}}$  if  $s_i s_{i-1} \le 0$ .
- $f_0' = \frac{3}{2} s_0 \frac{1}{2} f_1'$  and  $f_N' = \frac{3}{2} s_{N-1} \frac{1}{2} f_{N-1}'$  at the end points.
- 13. Shape-Preserving Knot-based  $C^2$  Cubic: Ideas are taken from the awesome paper by Pruess (1993). The basic idea is to take the interval  $[x_i, x_{i+1}]$ , and partition it into 3 parts by locating the two knots at  $\xi_i = x_i + \sigma_i h_i$ , and  $\eta_i = x_{i+1} \tau_i h_i$ . Evolve the criteria for the selection of  $\tau_i$  and  $\tau_i$  (and, of course, their corresponding responses) such that the local spline has shape-preserving feature, and avoids being global (i.e., preserves locality).
  - Using the above notations, the basic equations are:

• 
$$f(x) = f(x_i) + [x - x_i]f'(x_i) + [x - x_i]^2 \frac{f''(x_i)}{2} + [x - x_i]^3 \frac{f'''(x_i)}{6}$$
 for  $x \in [x_i, \xi_i].$ 

• 
$$f(x) = f(\xi_i) + [x - \xi_i]f'(\xi_i) + [x - \xi_i]^2 \frac{f''(\xi_i)}{2} + [x - \xi_i]^3 \frac{f'''(\xi_i)}{6}$$
 for  $x \in [\xi_i, \eta_i].$ 

• 
$$f(x) = f(\eta_i) + [x - \eta_i] f'(\eta_i) + [x - \eta_i]^2 \frac{f''(\eta_i)}{2} + [x - \eta_i]^3 \frac{f'''(\eta_i)}{6}$$
 for  $x \in [\eta_i, x_{i+1}].$ 

- The corresponding  $C^2$  maintenance solution then becomes (in terms of  $f'(x_i)$ ,  $f''(x_i)$ ,  $\sigma_i$ , and  $\tau_i$ , whose specification will then complete the inference):
  - $f(\xi_i) = f(x_i) + \sigma_i h_i f'(x_i) + \frac{\sigma_i^2 h_i^2}{6} \{ 2f''(x_i) + f''(\xi_i) \}.$
  - $f(\eta_i) = f(x_{i+1}) + \tau_i h_i f'(x_{i+1}) + \frac{\tau_i^2 h_i^2}{6} \{ 2f''(x_{i+1}) + f''(\eta_i) \}.$
  - $f'(\xi_i) = f'(x_i) + \frac{\sigma_i h_i}{2} \{f''(x_i) + f''(\xi_i)\}.$
  - $f'(\eta_i) = f'(x_{i+1}) \frac{\tau_i h_i}{2} \{ f''(x_{i+1}) + f''(\eta_i) \}.$
  - $f''(\xi_i) = \frac{6s_i 2(2 + \sigma_i \tau_i)f'(x_i) 2(1 \sigma_i + \tau_i)f'(x_{i+1}) \sigma_i h_i(2 \tau_i)f''(x_i) + \tau_i h_i(1 \sigma_i)f''(x_{i+1})}{h_i(1 \tau_i)}$

.

$$f''(\eta_i) = \frac{-6s_i + 2(1 + \sigma_i - \tau_i)f'(x_i) + 2(2 - \sigma_i + \tau_i)f'(x_{i+1}) + \sigma_i h_i (1 - \tau_i)f''(x_i) - \tau_i h_i (2 - \sigma_i)f''(x_{i+1})}{h_i (1 - \sigma_i)}$$

• 
$$f^{\prime\prime\prime}(x_i) = \frac{f^{\prime\prime}(\xi_i) - f^{\prime\prime}(x_i)}{\sigma_i h_i}$$
.

• 
$$f'''(\xi_i) = \frac{f''(\eta_i) - f''(\xi_i)}{(1 - \sigma_i - \tau_i)h_i}$$
.

• 
$$f'''(\eta_i) = \frac{f''(x_{i+1}) - f''(\eta_i)}{\tau_i h_i}$$
.

• Choice of  $f'(x_i)$  and  $f''(x_i)$ :  $f'(x_i)$  and  $f''(x_i)$  may be generated using typical generation schemes (e.g., using the Fritsch and Butland (1984) algorithm).

- The Preuss Inequalities: It is specified as follows. Set
  - $\beta_i = sign(s_i s_{i-1}); R_{2i-1} = 6s_i 4f_i' 2f_{i+1}'; R_{2i} = 2f_i' + 4f_{i+1}' 6s_i$
  - If  $\beta_i R_{2i-1} \ge 0$  and  $\beta_i R_{2i-1} \ge 0$ , you are done, since the chosen  $f_i$ ' and  $f_i$ '' also preserve convexity you can go and set the second derivatives, and set  $\tau_i$  and  $\sigma_i$ .
- Mismatch in the Preuss Inequalities: If the Preuss inequalities are not met,  $f_i$ ' and  $f_i$ '' need to be modified such that  $f_i$ '  $\in$   $[c_i, d_i]$  where  $c_i, d_i$  are obtained using the double sweep algorithm below.
- Preuss (1993) Double Sweep: First find  $a_i$  and  $b_i$  from the following regimes:

• If 
$$\beta_i > 0$$
,  $\beta_{i+1} > 0$ ,  $a_i = \max\left(s_i, \frac{3s_i - b_i}{2}\right)$ ;  $b_i = 3s_i - 2a_i$ .

• If 
$$\beta_i < 0, \beta_{i+1} > 0$$
,  $a_i = \max\left(3s_i - 2b_i, \frac{3s_i - b_i}{2}\right)$ ;  

$$b_i = \max\left(3s_i - 2a_i, \frac{3s_i - a_i}{2}\right).$$

• If 
$$\beta_i > 0$$
,  $\beta_{i+1} > 0$ ,  $a_i = \max(s_{i+1}, 3s_i - 2b_i)$ ;  $b_i = \frac{3s_i - a_i}{2}$ .

- Finally the  $a_0$  and  $b_0$  initializations are set from:
  - If  $\beta_0 > 0$ ,  $\beta_1 > 0$ ,  $a_0 = 3s_0 2b_0$ ;  $b_0 = s_0$ .
  - If  $\beta_0 < 0, \beta_1 < 0, \ a_0 = s_0$ ;  $b_0 = 3s_0 2s_1$ .
  - Preuss (1993) Backward Sweep for  $c_i, d_i$ : First set  $s_N' = f_N' = \frac{a_N + b_N}{2}$ , then set  $c_i, d_i$  using the following:

o If 
$$\beta_i > 0$$
,  $\beta_{i+1} > 0$ , then  $c_i = 3s_i - f_{i+1}'$ , and  $d_i = \frac{3s_i - f_{i+1}'}{2}$ .

$$\text{o} \quad \text{If } \beta_i < 0, \beta_{i+1} > 0 \text{, then } c_i = \max \left[ 3s_i - 2f_{i+1}', \frac{3s_i - f_{i+1}'}{2} \right], \text{ and }$$

$$d_i = \min \left[ 3s_i - 2f_{i+1}', \frac{3s_i - f_{i+1}'}{2} \right].$$

- o If  $\beta_i < 0$ ,  $\beta_{i+1} < 0$ , then  $c_i = \frac{3s_i f_{i+1}}{2}$ , and  $d_i = 3s_i 2f_{i+1}$ .
- Preuss (1993) Setting 2<sup>nd</sup> Derivatives:  $f_i'' = \beta_i \min \left[ \frac{\beta_i R_{2i-1}}{h_i}, \frac{\beta_i R_{2i-2}}{h_{i-1}} \right]$ .
- Preuss (1993) Final Step Setting  $\tau_i$  and  $\sigma_i$ : Setting  $\tau_i = \sigma_i = \frac{1}{3}$ , verify the following inequalities:

$$\circ \quad \beta_i [4f_i' + 2f_i'' + h_i f_i'' \tau_i (2 - \tau_i) - h_i f_{i+1}'' \tau_i (1 - \tau_i)] \le 6\beta_i s_i$$

$$\circ \quad \beta_{i+1} \left[ 2f_i' + 4f_i'' + h_i f_i'' \tau_i (1 - \tau_i) - h_i f_{i+1}'' \tau_i (2 - \tau_i) \right] \le 6\beta_{i+1} s_i$$

o If these inequalities are satisfied, then you have your  $f_i$ ',  $f_i$ '',  $\tau_i$ , and  $\sigma_i$ . Otherwise, reduce  $\tau_i$  and  $\sigma_i$  till they are satisfied.

# **Space Curves and Loops**

- 1. Space Curve Reproduction: Here is one way to construct loops that are not possible using the ordered variates, i.e.,  $x_1 < x_2 < ... < x_n$ .
  - If the ordering  $x_1 < x_2 < ... < x_n$  is switched out in favor of the DAG  $\{x_j, y_j\}$ , where the DAG vertices correspond to the loop trace, normal splines may be used to represent space curve loops.
- 2. Second Degree Parameterization: However, on using a second-degree parameterization of x and y such as  $x = f_X(u)$  and  $y = f_Y(u)$ , it may be possible to enforce the order  $u_1 < u_2 < ... < u_n$ . The corresponding control points are  $[u_1, x_1] . [u_n, x_n]$  and  $[u_1, y_1] . [u_n, y_n]$ .
  - a. Side effect of this is that you need to work on two pairs of splines one each for  $x = f_X(u)$  and  $y = f_Y(u)$ .
  - b. This can offer additional customization and freedom in the design of the surface, at the expense of computing additional splines.

- 3. Closed Loops: Further, if the start/end points coincide, this corresponds to a closed loop that satisfies the  $C^2$  continuity criterion.
  - a. This also implies that no extra head/tail  $\mathbf{C}^1$  slope specifications are required.

# **Spline Segment Calibration**

### Introduction

- 1. <u>Spline Segment Calibrator</u>: For a given segment, its calibration depends only on the segment local value set the other inputs come from the prior segments (except in the case of "left-most" segment, whose full set of inputs will have to be extraneously specified).
- Bayesian Techniques in Spline Calibration: Frequentist and Bayesian techniques such as MLE and MAP regression ought to be possible in the calibration of the spline segment/span coefficients.
- 3. <u>Main Calibration Inputs Modes</u>: Here we consider the following segment calibration input modes: a) Smoothing Best fit Splines, and b) Segment Best Fit Response Inputs with Constraints.

# **Smoothing Best Fit Splines**

- 1. <u>Definition</u>: Here the treatment is limited to within a segment. In this, the segment coefficients are calibrated to the following inputs:
  - Truthness Constraints.
  - Smoothness  $C^k$ .
  - Penalizing Segment Smoother.
  - Penalizing Segment Weighted Fitness Match (in the least-squared sense).

#### 2. Nomenclature:

- $p \Rightarrow 0,...,q-1 \Rightarrow$  Weighted fitness penalizer match points
- $i \Rightarrow 0,...,n-1 =$  Segment Basis Functions  $j \Rightarrow 0,...,n-1$
- m =>Roughness Penalty Match Derivative Order

- $r \Rightarrow r$  Separation
- $k \Rightarrow C^k$  Continuity

### 3. Spline Set Setup:

- Gross Penalizer = Best Fit Penalizer + Curvature Penalizer
- $\bullet \qquad \mathfrak{R} = \frac{1}{q} \, \mathfrak{R}_F + \lambda \mathfrak{R}_C$
- $\bullet \quad \mathfrak{R}_F = \sum_{p=0}^{q-1} W_p (y_p Y_p)^2$
- $\bullet \quad \mathfrak{R}_C = \int_{x_l}^{x_{l+1}} \left( \frac{\partial^m y}{\partial x^m} \right)^2 dx$
- Spline Response Setup =>  $y = \sum_{i=0}^{n-1} \beta_i f_i(x)$ ,  $y_p = \sum_{i=0}^{n-1} \beta_i f_i(x_p)$ , and

$$\frac{\partial^m y}{\partial x^m} = \sum_{i=0}^{n-1} \beta_i \frac{\partial^m f_i(x)}{\partial x^m}.$$

### 4. <u>Best Fit Penalizer Setup</u>:

- First Derivative =>  $\frac{\partial \Re_F}{\partial \beta_r} = 2 \sum_{p=0}^{q-1} W_p f_r (x_p) \left\{ \sum_{i=0}^{n-1} \beta_i f_i(x_p) Y_p \right\} = 0$ .
- Second Derivative =>  $\frac{\partial^2 \mathfrak{R}_F}{\partial \beta_r^2} = 2 \sum_{p=0}^{q-1} W_p f_r^2(x_p) > 0$ , so  $\mathfrak{R}_F$  has a minimum.

### 5. Curvature Penalizer Setup:

- First Derivative =>  $\frac{\partial \Re_C}{\partial \beta_r} = \sum_{i=0}^{n-1} \beta_i \int_{x_i}^{x_{i+1}} \left( \frac{\partial^m f_i}{\partial x^m} \right) \left( \frac{\partial^m f_r}{\partial x^m} \right) dx = 0$ .
- Second Derivative =>  $\frac{\partial^2 \Re_C}{\partial \beta_r^2} = 2 \int_{x_r}^{x_{r+1}} \left( \frac{\partial^m f_r}{\partial x^m} \right)^2 dx > 0$ , so  $\Re_C$  has a minimum.

### 6. <u>Second Derivative</u>:

a. 
$$\frac{\partial^{2} \Re}{\partial \beta_{r}^{2}} = \frac{1}{q} \frac{\partial^{2} \Re_{F}}{\partial \beta_{r}^{2}} + \lambda \frac{\partial^{2} \Re_{C}}{\partial \beta_{r}^{2}} = 2 \left\{ \frac{1}{q} \sum_{p=0}^{q-1} W_{p} f_{r}^{2} \left(x_{p}\right) + \lambda \int_{x_{l}}^{x_{l+1}} \left[ \frac{\partial^{m} f_{r}}{\partial x^{m}} \right]^{2} dx \right\} > 0!$$

# 7. <u>Joint Linearized Minimizer Setup</u>:

$$\bullet \quad \frac{\partial \Re}{\partial \beta_r} = \sum_{i=0}^{n-1} \beta_i \left\{ \frac{1}{q} \sum_{p=0}^{q-1} W_p f_i(x_p) f_r(x_p) + \lambda \int_{x_i}^{x_{i+1}} \left[ \frac{\partial^m f_i}{\partial x^m} \right] \left[ \frac{\partial^m f_r}{\partial x^m} \right] dx \right\} - \frac{1}{q} \sum_{p=0}^{q-1} W_p f_r(x_p) Y_p = 0$$

- 8. Number of Equations/Unknowns Review:
  - a. For intermediate segments, the following equations determine the unknowns:
    - i. Number of Continuity Constraints => k
    - ii. Number of Left/Right Node Values => 2
    - iii. Number of Roughness Penalizer Constraint => at least 1
    - iv. Thus, minimal number of degrees of freedom on a per-segment basis: k+3. This will be the number of "free" parameters we will use for to extract for each segment.
  - b. For left most segments, the following equations determine the unknowns:
    - i. Number of Left/Right Node Values => 2
    - ii. Number of Roughness Penalizer Constraint => at least 1
    - iii. Thus, for the set of k+3 parameters, the number of undetermined parameters: k
  - c. For the span as a whole, the number of degrees of freedom/undetermined parameters is k. You may determine:
    - i. The right-most second derivative, AND
    - ii. Possibly, the left-most second derivative
    - iii. For k, this will complete the set of undetermined coefficients.

# **Segment Best Fit Response with Constraint Matching**

- 1. <u>Purpose</u>: Here we assume that a linear transform exists the hidden state quantification metric and the measurement manifest metric.
- 2. <u>Caveat with the Segment-wise Representation</u>: Optimizing on certain constraints (such as multi-segment constraints) now ends up producing a highly non-sparse, dense matrix. This is simply a reflection on the multi-segment spanning nature of the constraint and the eventual optimization.

3. Constraint and Least-Square Spec:  $S_p = \hat{C}_p - C_p$  where  $\hat{C}_p = \sum_{s=0}^{t_p-1} \gamma_s \hat{y}_s$  and  $\hat{y}_s = \sum_{i=0}^{n-1} \beta_i f_i(x_s)$ . Note that when the hidden state quantification metric is identically the same as the measurement manifest metric,  $\gamma_s = 1$  and  $t_p = 1$ . This corresponds to computing the least-square minimization over the observations.

- 4. Constraint Formulation Development:  $\hat{C}_p = \sum_{i=0}^{n-1} \beta_i \sum_{s=0}^{t_p-1} \gamma_s f_i(x_s)$ , or  $\hat{C}_p = \sum_{i=0}^{n-1} \beta_i G_{ip}$ , where  $G_{ip} = \sum_{s=0}^{t_p-1} \gamma_s f_i(x_s)$ . The parallel between this and the original least-squares formulation can now be extended in a straightforward manner.
- 5. Weighted Constrained LSM:

• 
$$S_p = \hat{C}_p - C_p = \sum_{i=0}^{n-1} \beta_i G_{ip} - C_p$$

• 
$$S_p^2 = \beta_k^2 G_{kp}^2 + 2\beta_k G_{kp} \left[ \sum_{i=0,i\neq k}^{n-1} \beta_i G_{ip} - C_p \right] + \left[ \sum_{i=0,i\neq k}^{n-1} \beta_i G_{ip} - C_p \right]^2$$

6. Optimization of  $S^2$ :

$$\bullet S^{2} = \frac{1}{N} \left\{ \beta_{k}^{2} \sum_{p=0}^{q-1} W_{p} G_{kp}^{2} + 2\beta_{k} \sum_{p=0}^{q-1} W_{p} G_{kp} \left[ \sum_{i=0, i \neq k}^{n-1} \beta_{i} G_{ip} - C_{p} \right] + \sum_{p=0}^{q-1} W_{p} \left[ \sum_{i=0, i \neq k}^{n-1} \beta_{i} G_{ip} - C_{p} \right]^{2} \right\}$$

$$\bullet \quad \frac{\partial (S^2)}{\partial \beta_k} = 0 \Rightarrow \sum_{i=0}^{n-1} \beta_i \sum_{p=0}^{q-1} W_p G_{ip} G_{kp} = \sum_{p=0}^{q-1} W_p G_{kp} C_p$$

• 
$$\frac{\partial^2 (S^2)}{\partial \beta_k^2} = \sum_{p=0}^{q-1} W_p G_{kp}^2 \ge 0$$
 for  $W_p \ge 0$ , thus the extremum is a minimum.

# **Spline Jacobian**

### Introduction

- 1. Chain Rule vs. Matrix Operations of Linear Basis Function Combination: When it comes to extracting variate Jacobian of coefficients from boundary inputs, these are absolutely equivalent in fact, the coefficient Matrix is in reality a Jacobian itself.
  - Matrix entry as a Jacobian => Every entry of the Matrix A where AX = Y is actually a Jacobian entry, i.e.,  $A_{ij} = \frac{\partial Y_i}{\partial X_j}$ .
- 2. Self-Jacobian: Given an ordered pair  $\{x_i, y_i\}$  that needs to be interpolated/splined across, the self-Jacobian is defined as the vector  $\frac{\partial y(x)}{\partial y(x_i)}$ . More generally, the self-Jacobian may be defined as  $\frac{\partial y(x)}{\partial I_i}$  where  $I_j$  is an input.
  - O Self-Jacobian tells you the story of sensitivity/perturbability of the interpolant (y) on non-local points through  $I_j$ , since the  $C^k$  transmission occurs through  $I_j$ . Within a single segment, quadratic and greater splines cause fairly non-banded, dispersed Jacobians, indicating that the impact is non-local; linear splines produce simple banded/tri-diagonal Jacobians; and tension splines produce a combination of the two depending on the tension parameter (and therefore dense within the segment).
  - Obviously Jacobian of any function F(y(x)) is going to be dependent on the self-Jacobian  $\frac{\partial y(x)}{\partial I_i}$  because of the chain rule.

# **Optimizing Spline Basis Function Jacobian**

- 1. Coefficient- Value Micro-Jacobian: FA = Y where
  - A is the matrix of the basis coefficients  $\{a_0,a_1,a_2,...,a_{r+1},...,a_{k+1},...,a_{n-1}\}$
  - Y is the matrix (column valued) of the values (RHS). In particular, it is the boundary segment calibration nodal values in the following order:

$$\left\{y_0, y_1, \left\|\frac{\partial y}{\partial x}\right\|_{x=0}, \dots, \left\|\frac{\partial^r y}{\partial x^r}\right\|_{x=0}, \dots, \left\|\frac{\partial^k y}{\partial x^k}\right\|_{x=0}, 0, \dots, 0\right\}$$

• F is the matrix of the coefficients of the basis function values and their derivatives. It is the following 2D Matrix:

$$0 \quad l = 0; j = 0,..n - 1 \Rightarrow F_{0j} = f_j(x = 0)$$

$$0 \quad l = 1; j = 0, ... n - 1 \Rightarrow F_{1j} = f_j(x = 1)$$

$$0 2 \le l \le k+1; j=0,...n-1 \Rightarrow F_{lj} = \left[\frac{\partial^{l-1} f_j}{\partial x^{l-1}}\right]_{x=0}$$

$$\circ \quad l \to k+2,...,n-1; j \to 0,...,n-1 \Longrightarrow Q_{l,j} \text{ where }$$

$$Q_{l,j} = \int_{x_j}^{x_{i+1}} \left[ \frac{\partial^m f_l(x)}{\partial x^m} \right] \left[ \frac{\partial^m f_j(x)}{\partial x^m} \right] dx.$$

2. <u>Coefficient-Value Micro-Jacobian</u>: Given FA = Y, the coefficient-value micro-Jack is  $\frac{\partial a_i}{\partial y_i} = [F^{-1}]_{ij}$ .

# Spline Input Quote Sensitivity Jacobian

- Segment Quote Jacobian: Formulation for quote Jacobian is different than those for
  the coefficient edge value Jacobian, since the former automatically figures in the
  design matrix in the sensitivity matrix extractor pseudo-calibration stage. Thus, the
  quote sensitivities are effectively external sensitivity constraints transmitted via the
  design matrix quote sensitivities.
- Quote Jacobian Matrix: The Quote Sensitivity coefficients are calibrated identically
  to that of the base coefficient sensitivities. This simply follows from the linearity of

the quote sensitivity formulation. The only area where there is non-linearity is in the product term  $\beta_i \alpha(q_c)$ , and that appears only at the constraint equations. Others are identically the same.

- 3. <u>Latent State Quote Sensitivity</u>: Spline Formulation of the Latent State automatically implies that the quote sensitivity of the latent state is restricted by the above, and is therefore also a spline in itself. This further implies that the boundary formulation is subject to the similar edge conditions as before.
- 4. <u>Terminology and Nomenclature</u>:

a. 
$$q_c \Rightarrow$$
 Input "Calibration Quotes"  $q_c \Rightarrow q_0,...,q_{d-1}$ 

b. 
$$n_{VM} =>$$
Number of explicit Input Node Value Matches

c. 
$$n_{CM}$$
 => Number of explicit Input Constraint Value Matches

d. 
$$n_{DM} =>$$
Number of explicit Input Derivative Value Matches

e. 
$$n_{PM}$$
 => Number of explicit Input Penalty Value Matches

- 2. Explicit Input-to-Response Match: This emanates from the  $C^0$  node match continuity criterion:  $\sum_{i=0}^{n-1} \beta_i f_i(x_j) = F_j \Rightarrow \sum_{i=0}^{n-1} f_i(x_j) \frac{\partial \beta_i}{\partial a} = \frac{\partial F_j}{\partial a} \text{ for } j = 0,...,n_{VM} 1.$
- 3. Explicit Input-to-Constraint Match:  $\sum_{i=0}^{n-1} \beta_i \gamma_{ij} = V_j \Rightarrow \sum_{i=0}^{n-1} \frac{\partial \left[ \beta_i \gamma_{ij} \right]}{\partial q_c} = \frac{\partial V_j}{\partial q_c} \text{ for }$   $j = n_{VM}, ..., n_{CM} 1. \text{ This may be re-written as } \sum_{i=0}^{n-1} \gamma_{ij} \frac{\partial \beta_i}{\partial q_c} = \frac{\partial V_j}{\partial q_c} \sum_{i=0}^{n-1} \beta_i \frac{\partial \gamma_{ij}}{\partial q_c}.$
- 4. Explicit Input-to-Derivative Match: This emanates from the  $C^k$  continuity criterion:  $\sum_{i=0}^{n-1} \beta_i \left| \frac{\partial f_i(x)}{\partial x} \right|_{x=x_j} = \Diamond_j \Rightarrow \sum_{i=0}^{n-1} \frac{\partial \beta_i}{\partial q_c} \left| \frac{\partial f_i(x)}{\partial x} \right|_{x=x_j} = \frac{\partial \Diamond_j}{\partial q_c} \text{ for } j = n_{CM}, ..., n_{DM} 1.$
- 5. Explicit Input-to-Penalizer Match: This emanates from the criterion for the curvature and length penalties:  $\sum_{i=0}^{n-1} \beta_i C_{ij} = P_j \Rightarrow \sum_{i=0}^{n-1} C_{ij} \frac{\partial \beta_i}{\partial q_c} = \frac{\partial P_j}{\partial q_c} \text{ for } j = n_{DM}, ..., n_{PM} 1.$

# **Shape Preserving Spline**

## **Shape Preserving Tension Spline**

- Integrated vs. Partitioned Shape Controller: Integrated Shape Controllers apply shape control on a basis function-by-basis function basis (certain basis functions such as flat/linear polynomial functions need no shape controller applied on them).
   Partitioned shape controllers apply shape control on a segment-by-segment basis.
- 2. Shape Controller Parameter Types:
  - Specified extraneously as part of the basis function formulation itself (e.g., hyperbolic/exponential tension splines)
  - Specified by over-determination of the basis function set (e.g.,  $\nu$  splines)
  - Specified by using a shape controller basis set that is de-coupled from the model basis function set (e.g., partitioned rational splines)
- 3. Shape Control as part of Basis Function formulation:
  - Each basis function is typically formulated as a linear interpolant of a particular  $r^{th}$  derivative across a segment, i.e.,  $\frac{\partial^r y}{\partial x^r} \sigma^r y$  is proportional to  $x^1$  in that segment.
  - Advantage is that you can control the switch between the  $r^{th}$  derivative and the  $0^{th}$  derivative of y by controlling  $\sigma$ .
  - You can also explicitly formulate it to achieve  $C^k$  continuity across segments and k can vary independently of r.
- 4. Drawbacks of Shape Control as part of Basis Function formulation:
  - ullet may not map well to the curvature/shape departure minimization metrics.
  - The formulation constraint restricts the choice of basis functions, giving rise to
    possibly unwieldy ones (troubles with exponential/hyperbolic functions are welldocumented).
- 5. Shape Control using over-determined Basis Function Set:

- Choose any set of basis Functions (e.g., based on simplicity/ease of use/model propriety).
- Over-specify the set so that additional coefficients are available for explicit and flexible shape control
- Explicit shape control formulation => this comes out a minimization exercise of a "shape departure penalty" function.

#### 6. Drawbacks of Shape Control using Over-determined Basis Function formulation:

- Ease of use, more model/physics targeted, but comes with extra complexity that trades in flexibility
- Formulation Complexity => Incorporating variational techniques for enforcing compliance by penalizing shape departure.
- Functional implementation complexity
- Jacobian estimation complexity => Now  $n \times n$  basis functions for which we need Jacobian.
- Algorithmic complexity => Need more robust basis inversion/linearization techniques.

#### 7. Potentially Best of Both – Partitioned Basis and Shape Control:

- Basis function set chosen from physics and other considerations
- Shape Control achieved using targeted Shape Controllers
- Used in conjunction with over-determined/other shape control techniques.

#### 8. Drawbacks of Using Partitioned Basis Functions:

- Choice of shape controllers crucial and non-trivial they have to satisfy the segment edge and shape variational constraints
- Need clear and well-specified formulations to match/satisfy the appropriate metrics of shape preservation
- Formulation Complexity all calibrations and Jacobians need to incorporate the partitioned basis right during the formulation stage
  - When dealing with snipping/clipping segments, shape controllers operate best at the global level (i.e., at the span/stretch basis). Shape controller smoothness continuity will therefore be ensured, but requires careful

formulation at the local/global switch part (i.e., translation of the derivatives using the span/segment scales has to be done carefully).

- 9. <u>Partitioned vs. Integrated Tension Splines</u>: Partitioned splines are designed such that the interpolant functional and the shape control functional are separated by formulation (e.g., rational splines). Integrated tension splines are formulated such that the shape preservation is an inherent consequence of the formulation, and there is no separation between the interpolant and the shape control functionality.
  - Customization is easier with partitioning on either the control design or the shape preservation dimension.
- 10. Explicit Shape Preservation Control in Partitioned Splines:  $y = \frac{\alpha}{\beta}$ , where  $\alpha$  is the interpolant, and  $\beta$  is the shape controller. Typically  $\alpha$  is determined (among other things) by the continuity criterion  $C^k$ , and  $\beta$  contains an explicit design parameter for shape control (for e.g.,  $\lambda$  in the case of rational splines).
- 11. Shape Control Design: Asymptotically, depending on the shape design parameter  $\lambda$ ,  $\frac{\alpha}{\beta}$  should switch between linear and polynomial (i.e., typically cubic Qu and Sarfraz (1997)). Further, design  $\beta$  such that  $\beta_0 = \beta_1 = 1$ , so that  $y_0 = \alpha_0$  and  $y_1 = \alpha_1$

12. Rational Cubic Spline Formulation:

- Rational functions under tension was introduced by Spath (1974), and formulation expanded in the general tension setting by Preuss (1976).
- $y = \frac{a + bx + cx^2 + dx^3}{1 + \lambda x(1 x)} = \frac{\alpha}{\beta}$ , where  $\alpha = a + bx + cx^2 + dx^3$ , and  $\beta = 1 + \lambda x(1 x)$ (Delbourgo and Gregory (1983), Delbourgo and Gregory (1985a), Delbourgo and Gregory (1985b), Delbourgo (1989)).
- $\lambda \to 0$  makes it cubic, and  $\lambda \to \infty$  makes it linear.
- 13. Rational Cubic Spline Coefficients:
  - $a = 1.y_0 + 0.y_1 + 0.y_0' + 0.y_0''$
  - $b = \lambda y_0 + 0 y_1 + 1 y_0' + 0 y_0''$

• 
$$c = -\lambda y_0 + 0 y_1 + \lambda y_0' + \frac{1}{2} y_0''$$

• 
$$d = -1.y_0 + 1.y_1 + [-(1+\lambda)]y_0' + (-\frac{1}{2})y_0''$$

## 14. Rational Cubic Spline Derivatives:

$$\bullet \quad \alpha = a + bx + cx^2 + dx^3$$

$$\bullet \quad \frac{d\alpha}{dx} = b + 2cx + 3dx^2$$

$$\bullet \quad \frac{d^2\alpha}{dx^2} = 2c + 6dx$$

$$\bullet \quad \beta = 1 + \lambda x (1 - x)$$

$$\bullet \quad \frac{d\beta}{dx} = \lambda (1 - 2x)$$

$$\bullet \quad \frac{d^2\beta}{dx^2} = -\lambda$$

$$\bullet \quad \frac{dy}{dx} = \frac{\beta \frac{d\alpha}{dx} - \alpha \frac{d\beta}{dx}}{\beta^2}$$

$$\bullet \quad \frac{d^2y}{dx^2} = \frac{\beta^2 \frac{d^2\alpha}{dx^2} - \alpha\beta \frac{d^2\beta}{dx^2} + 2\alpha \left(\frac{d\beta}{dx}\right)^2 - 2\beta \frac{d\alpha}{dx} \frac{d\beta}{dx}}{\beta^2}$$

# 15. <u>Designing</u> $\lambda_i$ for the Segment Inflection/Extrema Control:

- If there are "physics" hints, the segment  $\lambda_i$  can be designed to push out/pull in the inflections and/or extrema out of (or into) the segment.
- Monotonizing Parameters for Rational Splines (Gregory (1984), Gregory (1986))

=> 
$$\lambda_i = \mu_i + [f'(x_i) + f'(x_{i+1})] \frac{x_{i+1} - x_i}{y_{i+1} - y_i}$$
, again for  $x_i < x < x_{i+1}$ .

- $\mu_i \ge -3$  makes it monotone in this segment.
- $\mu_i = -2$  produces a rational quadratic.
- Convergence is  $\Theta(h^4)$  in all cases.

- 16. Co-convex choice for  $\underline{\lambda}$ : A similar analysis can be done to make the spline co-convex, but the corresponding formulation requires a non-linear solution for  $\lambda_i$ .
- 17. Generalized Shape Controlling Interpolator: Given a pair of points  $\{x_1, y_1\} \rightarrow \{x_2, y_2\} \Rightarrow \{0, y_1\} \rightarrow \{1, y_2\}$ , a  $C^0$  spline  $S_0$ , and a  $C^k$  spline  $S_k$ , we define a shape controlling interpolator spline  $S_C$  by  $S_C(x) \propto \frac{1}{\left[S_k(x) S_0(x)\right]^2}$ , with the constraints  $S_C(x = 0) = S_C(x = 1) = 1$ .
  - Rational Shape Controller described earlier meets these requirements.
- 18. Generically Partitioned Spline Derivative:

• 
$$y(x) = \alpha(x)\beta(x)$$

$$\bullet \quad \frac{\partial y}{\partial x} = \frac{\partial \alpha}{\partial x} \beta + \alpha \frac{\partial \beta}{\partial x}$$

• 
$$\frac{\partial^2 y}{\partial x^2} = \frac{\partial^2 \alpha}{\partial x^2} \beta + 2 \frac{\partial \alpha}{\partial x} \frac{\partial \beta}{\partial x} + \alpha \frac{\partial^2 \beta}{\partial x^2}$$

• More generally 
$$\frac{\partial^n y}{\partial x^n} = \sum_{r=0}^n {\binom{n-r}{2r}} \frac{\partial^{n-r} \alpha}{\partial x^{n-r}} \frac{\partial^r \beta}{\partial x^r}$$

19. Partitioned Interpolating Spline Coefficient: Given  $\beta_0 = \beta_1 = 1$ ,

• 
$$y_0 = \alpha_0$$

• 
$$y_1 = \alpha_1$$

• 
$$\left[\frac{\partial y}{\partial x}\right]_{x=0} = \left[\frac{\partial \alpha}{\partial x}\right]_{x=0} \left[\beta\right]_{x=0} + \left[\alpha\right]_{x=0} \left[\frac{\partial \beta}{\partial x}\right]_{x=0} \Rightarrow \left[\frac{\partial \alpha}{\partial x}\right]_{0} = \left[\frac{\partial y}{\partial x}\right]_{0} - \alpha_{0} \left[\frac{\partial \beta}{\partial x}\right]_{0} = \left[\frac{\partial \beta}{\partial x}\right]_{0} + \left[\alpha\right]_{0} \left[\frac{\partial \beta}{\partial x}\right]_{0} = \left[\frac{\partial \beta}{\partial x}\right]_$$

• Likewise, 
$$\left| \frac{\partial^2 \alpha}{\partial x^2} \right|_0 = \left| \frac{\partial^2 y}{\partial x^2} \right|_0 - \alpha_0 \left| \frac{\partial^2 \beta}{\partial x^2} \right|_0 - 2 \left| \frac{\partial \alpha}{\partial x} \right|_0 \left| \frac{\partial \beta}{\partial x} \right|_0$$

• Partitioned input micro-Jack for cubic interpolator:

$$\circ \quad a = \{1\}.y_0 + \{0\}.y_1 + \{0\}.y_0' + \{0\}.y_0''\}$$

$$c = \left[ \left( \left| \frac{\partial \beta}{\partial x} \right|_{0} \right)^{2} - \frac{1}{2} \left| \frac{\partial^{2} \beta}{\partial x^{2}} \right|_{0} \right] y_{0} + 0.y_{1} + \left[ -\left| \frac{\partial \beta}{\partial x} \right|_{0} \right] y_{0}' + \frac{1}{2}.y_{0}''$$

$$c = \left[ \frac{1}{2} \left| \frac{\partial^{2} \beta}{\partial x^{2}} \right|_{0} + \left| \frac{\partial \beta}{\partial x} \right|_{0} - \left( \left| \frac{\partial \beta}{\partial x} \right|_{0} \right)^{2} - 1 \right] y_{0} + 1.y_{1} + \left[ \left| \frac{\partial \beta}{\partial x} \right|_{0} - 1 \right] y_{0}' + \left[ -\frac{1}{2} \right] y_{0}''$$

- 20. Interpolating Polynomial Splines of Degree n: Given  $y = \sum_{i=0}^{n} \alpha_i x^i$ ,  $x \in [0,1)$ 
  - Polynomial Basis Series for Representation => Taylor series uses the polynomial basis series for representation, and is popular because of the reasons below (other basis may be more cognitive, and derivative representation using them may be more intuitive as well).
    - i. Mathematical simplicity
    - ii. Completeness.
  - Native link of polynomials to derivatives => Given that derivatives are natively
    linked polynomial basis function representations, all the lower degree polynomial
    basis functions (i.e., degree < derivative order) get eliminated, thus only allowing
    the higher order to survive.</li>

• Polynomial 
$$C^k$$
 Derivative  $\Rightarrow \frac{\partial^r y}{\partial x^r} = \sum_{i=0}^n \alpha_i \frac{i!}{(i-r)!} x^{i-r} = \sum_{i=r}^n \alpha_i \frac{i!}{(i-r)!} x^{i-r}$ 

- $\alpha_0 = y_0$
- $\alpha_r = \frac{1}{r!} \left[ \frac{\partial^r y}{\partial x^r} \right]_{x=0}, \quad r \in [1, n-1]$
- $\bullet \quad \alpha_n = y_1 \sum_{i=0}^{n-1} \alpha_i = y_1 \sum_{r=0}^{n-1} \left\{ \frac{1}{r!} \left[ \frac{\partial^r y}{\partial x^r} \right]_{x=0} \right\}$
- 21. "Derivative Completeness" Nature of Polynomial Basis Function: One big advantage for polynomial basis functions is that they are "derivative complete" in the local as well as global sense, i.e., the k+1 basis polynomials are sufficient to uniquely determine the  $C^k$  continuity constraint. This is not true of non-polynomial basis functions (exponential basis functions, for e.g., need an infinite number of derivatives

for completely derivative coefficient determination), therefore their shape needs global determination.

## 22. Polynomial Interpolating Spline Coefficient micro-Jack:

$$\bullet \quad \frac{\partial \alpha_0}{\partial y_0} = 1, \frac{\partial \alpha_0}{\partial y_1} = 0, \left\{ \frac{\partial \alpha_0}{\partial \left[ \left[ \frac{\partial^r y}{\partial x^r} \right] \right]} \right\}_{x=0,0 \neq r} = 0$$

• 
$$\frac{\partial \alpha_k}{\partial y_0} = 1, \frac{\partial \alpha_k}{\partial y_1} = 0, \left\{ \frac{\partial \alpha_k}{\partial \left[ \left[ \frac{\partial^r y}{\partial x^r} \right] \right]} \right\}_{x=0} = \frac{1}{r!} \delta_{kr}$$

$$\bullet \quad \frac{\partial \alpha_n}{\partial y_0} = -1, \frac{\partial \alpha_n}{\partial y_1} = 1, \left\{ \frac{\partial \alpha_n}{\partial \left[ \left[ \frac{\partial^r y}{\partial x^r} \right] \right]} \right\}_{x=0,0 \neq r} = -\frac{1}{r!}$$

- 23. <u>Curvature Design in Integrated Tension Splines</u>: Cubic spline is interpolant on  $\frac{\partial^2 y}{\partial x^2}$  across the nodes, and linear spline is interpolant on y. Thus,  $\frac{\partial^2 y}{\partial x^2} \sigma^2 y$  (the tension spline interpolant) offers the tightness vs. curvature smoothness trade-off.
  - Tightness vs. Smoothness Generalization =>  $\frac{\partial^k y}{\partial x^k} \sigma^k y$  is linear in x, given k is even. Of course, for k = 2 this describes a tension spline (hyperbolic or exponential). Schweikert (1966) used k = 4 to improve the shape preservation characteristics.

## 24. Basis Function Interpolant:

•  $\frac{\partial^2 y}{\partial x^2} - \sigma^2 y$  that is linear in x is satisfiable only by hyperbolic and exponential basis splines.

- $\frac{\partial^4 y}{\partial x^4} \sigma^4 y$  that is linear in x is satisfiable by hyperbolic, exponential, or sinusoidal basis splines.
- More generally,  $\frac{\partial^n y}{\partial x^n} \sigma^n y$  that is linear in x, and where n = 4m + 2 and m = 0,1,... is satisfied only by hyperbolic and exponential splines.
- $\frac{\partial^n y}{\partial x^n} \sigma^n y$  that is linear in x, and where n = 4m and m = 0,1,... is satisfied only by hyperbolic, exponential, or sinusoidal splines.
- 25. <u>Integrated Tension Spline Types</u>: Sets containing both exponential and hyperbolic basis splines and a linear spline satisfy  $\frac{\partial^2 y}{\partial x^2} \sigma^2 y$ .
  - Exponential Basis Splines:  $\left\{1, x, e^{\frac{\alpha}{x_{i+1} x_i}}, e^{\frac{-\alpha}{x_{i+1} x_i}}\right\}$
  - Hyperbolic Basis Splines:  $\left\{1, x, \cosh\left(\frac{\sigma x}{x_{i+1} x_i}\right), \sinh\left(\frac{\sigma x}{x_{i+1} x_i}\right)\right\}$

## 26. Exponential Basis Functions:

• Base Segment Formulation =>

$$0 y = A + Bx + Ce^{\frac{\alpha}{x_1 - x_0}} + De^{-\frac{\alpha}{x_1 - x_0}}$$

$$\circ \quad y = \alpha + \beta \varepsilon + \gamma e^{\sigma \varepsilon} + \delta e^{-\sigma \varepsilon}$$

• Global <-> Local =>

$$\circ \quad \alpha = A + Bx_0$$

$$\circ \quad \beta = B(x_1 - x_0)$$

$$\circ \quad \gamma = Ce^{\frac{-\alpha x_0}{x_1 - x_0}}$$

$$\circ \quad \delta = De^{-\frac{\sigma x_0}{x_1 - x_0}}$$

• Local <-> Global =>

$$\circ \quad D = \delta e^{\frac{-\alpha x_0}{x_1 - x_0}}$$

$$\circ \quad C = \gamma e^{-\frac{\sigma x_0}{x_1 - x_0}}$$

$$\circ \quad B = \frac{\beta}{x_1 - x_0}$$

$$\circ \quad A = \alpha - \frac{\beta x_0}{x_1 - x_0}$$

• Co-efficient Calibration =>

$$\circ \quad \alpha = y_0 - \frac{y_0''}{\sigma^2}$$

$$\circ \quad \gamma = \frac{1}{2} \left[ \frac{y_0'' + \sigma(y_0 - \beta)}{\sigma^2} \right]$$

$$\circ \quad \delta = \frac{1}{2} \left[ \frac{y_0'' - \sigma(y_0' - \beta)}{\sigma^2} \right]$$

$$\circ \quad \beta = \frac{\sigma^2(y_1 - \alpha) - y_0 \cosh \sigma - \sigma y_0 \sinh \sigma}{\sigma(\sigma - \sinh \sigma)}$$

• Coefficient to Input Sensitivity Grid =>

$$\circ \quad \alpha = [1]y_0 + [0]y_1 + [0]y_0 - \left[\frac{1}{\sigma^2}\right]y_0$$

$$\circ \quad \beta = \left[ \frac{-\sigma}{\sigma - \sinh \sigma} \right] y_0 + \left[ \frac{\sigma}{\sigma - \sinh \sigma} \right] y_1 + \left[ \frac{-\sinh \sigma}{\sigma - \sinh \sigma} \right] y_0 + \left[ \frac{1 - \cosh \sigma}{\sigma (\sigma - \sinh \sigma)} \right] y_0$$

$$\circ \quad \gamma = \left[ \frac{1}{2(\sigma - \sinh \sigma)} \right] y_0 + \left[ \frac{-1}{2(\sigma - \sinh \sigma)} \right] y_1 + \left[ \frac{1}{2(\sigma - \sinh \sigma)} \right] y_0 + \left[ \frac{\sigma - 1 + \cosh \sigma - \sinh \sigma}{2\sigma^2(\sigma - \sinh \sigma)} \right] y_0$$

$$\circ \quad \delta = \left[\frac{-1}{2(\sigma - \sinh \sigma)}\right] y_0 + \left[\frac{1}{2(\sigma - \sinh \sigma)}\right] y_1 + \left[\frac{-1}{2(\sigma - \sinh \sigma)}\right] y_0 + \left[\frac{\sigma + 1 - \cosh \sigma - \sinh \sigma}{2\sigma^2(\sigma - \sinh \sigma)}\right] y_0$$

• Local Derivatives =>

$$\circ \quad \frac{\partial y}{\partial \varepsilon} = \beta + \sigma \left[ \gamma e^{\alpha \varepsilon} - \delta e^{-\alpha \varepsilon} \right]$$

$$\circ \frac{\partial^2 y}{\partial \varepsilon^2} = \sigma^2 \left[ \gamma e^{\alpha \varepsilon} + \delta e^{-\alpha \varepsilon} \right]$$

• Global <-> Local Derivatives =>

$$\circ \frac{\partial^3 y}{\partial x^3} = \frac{1}{(x_1 - x_0)^3} \frac{\partial^3 y}{\partial \varepsilon^3}$$

## 27. Hyperbolic Basis Functions:

• Base Segment Formulation =>

$$0 y = A + Bx + C \cosh\left(\frac{\sigma x}{x - x_0}\right) + D \sinh\left(\frac{\sigma x}{x - x_0}\right)$$

$$0 \quad y = \alpha + \beta \varepsilon + \gamma \cosh(\sigma \varepsilon) + \delta \sinh(\sigma \varepsilon)$$

• Global <-> Local =>

$$\circ \quad x = x_0 + \varepsilon (x_1 - x_0)$$

$$\circ \quad \varepsilon = \frac{x - x_0}{x_1 - x_0}$$

$$\circ \quad \alpha = A + Bx_0$$

$$\circ \quad \beta = B(x_1 - x_0)$$

$$\circ \quad \gamma = C \cosh\left(\frac{\sigma x_0}{x - x_0}\right) + D \sinh\left(\frac{\sigma x_0}{x - x_0}\right)$$

$$\circ \quad \delta = C \sinh\left(\frac{\sigma x_0}{x - x_0}\right) + D \cosh\left(\frac{\sigma x_0}{x - x_0}\right)$$

• Coefficient to Input Sensitivity Grid =>

$$\circ \quad \alpha = [1]y_0 + [0]y_1 + [0]y_0 + \left[\frac{-1}{\sigma^2}\right]y_0$$

$$\circ \quad \beta = \left[\frac{\sigma}{\sigma - \sinh \sigma}\right] y_0 + \left[\frac{-\sigma}{\sigma - \sinh \sigma}\right] y_1 + \left[\frac{\sinh \sigma}{\sigma - \sinh \sigma}\right] y_0 + \left[\frac{\cosh \sigma - 1}{\sigma(\sigma - \sinh \sigma)}\right] y_0$$

$$\circ \quad \gamma = [0]y_0 + [0]y_1 + [0]y_0 + \left[\frac{1}{\sigma^2}\right]y_0$$

$$\circ \quad \delta = \left[\frac{-1}{\sigma - \sinh \sigma}\right] y_0 + \left[\frac{1}{\sigma - \sinh \sigma}\right] y_1 + \left[\frac{-1}{\sigma - \sinh \sigma}\right] y_0 + \left[\frac{1 - \cosh \sigma}{\sigma^2 (\sigma - \sinh \sigma)}\right] y_0$$

• Local Derivatives =>

$$\circ \quad \frac{\partial y}{\partial \varepsilon} = \beta + \sigma [\gamma \sinh(\sigma \varepsilon) + \delta \cosh(\sigma \varepsilon)]$$

$$\circ \frac{\partial^2 y}{\partial \varepsilon^2} = \sigma^2 [\gamma \cosh(\sigma \varepsilon) + \delta \sinh(\sigma \varepsilon)]$$

$$\circ \frac{\partial^3 y}{\partial \varepsilon^3} = \sigma^3 [\gamma \sinh(\sigma \varepsilon) + \delta \cosh(\sigma \varepsilon)]$$

$$\circ \quad \frac{\partial^r y}{\partial \varepsilon^r} = \sigma^r \left[ \gamma \cosh(\sigma \varepsilon) + \delta \sinh(\sigma \varepsilon) \right] \text{ if r is even.}$$

$$\circ \quad \frac{\partial^r y}{\partial \varepsilon^r} = \beta \delta_{1r} + \sigma^r [\gamma \sinh(\sigma \varepsilon) + \delta \cosh(\sigma \varepsilon)] \text{ if r is odd.}$$

• Global <-> Local Derivatives =>

$$\circ \quad \frac{\partial y}{\partial x} = \frac{1}{\left(x_1 - x_0\right)} \frac{\partial y}{\partial \varepsilon}$$

$$\circ \frac{\partial^2 y}{\partial x^2} = \frac{1}{(x_1 - x_0)^2} \frac{\partial^2 y}{\partial \varepsilon^2}$$

$$\circ \frac{\partial^3 y}{\partial x^3} = \frac{1}{(x_1 - x_0)^3} \frac{\partial^3 y}{\partial \varepsilon^3}$$

- 28. Alternate specifications of the segment interpolation (Trojand (2011)). Renka (1987) provides techniques for setting  $\sigma$  under several circumstances:
  - o Finding  $\sigma$  when f is bound.
    - To get the minimum tension factor required we need to find the zeros of f' (Renka (1987)).
  - o Finding  $\sigma$  when f is bound.

- To get the minimum tension factor required we need to find the zeros of f' (Renka (1987)).
- $\circ$  Finding  $\sigma$  from the bound values of convexity/concavity (Renka (1987)).
- 29. Problems with Hyperbolic/Tension Splines:
  - Hyperbolic and exponential functions are time consuming to compute (Preuss (1976)), Lynch (1982)).
  - They are somewhat unstable to wide parameter ranges (Spath (1969), Sapidis, Kaklis, and Loukakis (1988)).
  - In certain cases, reasonable alternatives have been provided by  $\nu$  splines (Nielson (1974)) and rational splines.

# Shape Preserving $\nu$ Splines

- 1. <u>Generic v Spline Formulation</u>: Approach here is somewhat similar to Foley (1988), although different language/symbology.
  - p-set Basis Splines per each Segment.
  - n Data Points
  - Penalty of degree m
  - C<sup>k</sup> Continuity Criterion
  - Data Point Set:  $\{x_i, y_i\}$
  - Spline Objective Function:

$$\Lambda\left(\hat{\mu}, k, m, n, p, \overrightarrow{\lambda}\right) = \sum_{i=1}^{n-1} \left\{ \left[Y_i - \hat{\mu}_P(x_i)\right]^2 + \lambda_i \int_{x_1}^{x_{i+1}} \left[\frac{\partial^m \hat{\mu}_P(x)}{\partial x^m}\right]^2 dx \right\} + \left[Y_n - \hat{\mu}_P(x_n)\right]^2$$

- 2. Number of Unknowns Analysis: In the above, p > m, and  $m \le k$ .
  - Number of equations from the end points per segment => 2.
  - Number of equations from the coefficients determined by the  $C^k$  Continuity Criterion: k.

• Number of equations from the Shape Optimization Formulation:  $w \in [0, p-m+1]$ 

- Total number of equations: k + w + 2.
- Number of coefficients per segment  $\Rightarrow p+1$ .
- 3. <u>Node matching constraints</u>: Given that we are examining shape preserving splines, on applying the node match criterion  $Y_i = \stackrel{\circ}{\mu}_P(x_i)$  to  $\Lambda(\stackrel{\circ}{\mu}, k, m, n, p, \stackrel{\rightarrow}{\lambda})$  formulated

earlier, we get 
$$\Lambda_{NM}\left(\hat{\mu}, k, m, n, p, \overrightarrow{\lambda}\right) = \sum_{i=1}^{n-1} \left\{ \lambda_i \int_{x_i}^{x_{i+1}} \left[ \frac{\partial^m \hat{\mu}_P(x)}{\partial x^m} \right]^2 dx \right\}$$
 where

$$\Lambda_{NM}\left(\stackrel{\circ}{\mu},k,m,n,p,\stackrel{\rightarrow}{\lambda}\right)$$
 is the node matched Spline Objective Function.

4. <u>Generic Curvature Optimization Formulation</u>: Using the above, the curvature optimization for spline basis function inside a local segment i corresponds to

$$\Lambda_i = \int_{x_i}^{x_{i+1}} \left[ \frac{\partial^m \dot{\mu}(x)}{\partial x^m} \right]^2 dx.$$

5. <u>Generic Curvature Optimization Minimizer</u>: Given the basis function set

$$\hat{\mu}_{i}(x) = \sum_{j=0}^{n-1} \alpha_{ik} f_{j}(x), \quad \frac{\partial \Lambda_{i}}{\partial \alpha_{ik}} = 2 \sum_{j=0}^{n-1} \alpha_{ik} \int_{x_{i}}^{x_{i+1}} \left[ \frac{\partial^{m} f_{j}(x)}{\partial x^{m}} \right] \left[ \frac{\partial^{m} f_{k}(x)}{\partial x^{m}} \right] dx.$$

6. Generic Coefficient Constrained Optimization Setup:  $\frac{\partial \Lambda_i}{\partial \alpha_{ik}} = 0 \Rightarrow \sum_{j=0}^{n-1} \alpha_{ik} Q_{ijk} = 0$ 

where 
$$Q_{ijk} = \int_{x_i}^{x_{i+1}} \left[ \frac{\partial^m f_j(x)}{\partial x^m} \right] \left[ \frac{\partial^m f_k(x)}{\partial x^m} \right] dx$$
.

7. Polynomial Formulation for  $\Lambda_{NM}\left(\hat{\mu}, k, m, n, p, \overrightarrow{\lambda}\right)$ : For the set of polynomial basis

functions, we set 
$$\hat{\mu_p}(x) = \hat{\mu_i}(p,x) = \sum_{j=0}^p \alpha_{ij} x^j$$
 on a segment-by-segment basis.

• We also seek to optimize  $\Lambda_{NM}(\hat{\mu}, k, m, n, p, \vec{\lambda})$  on a per-segment basis by re-

casting 
$$\Lambda_{NM}(\hat{\mu}, k, m, n, p, \vec{\lambda})$$
 to  $\Lambda_i(k, m, p) = \int_{x_1}^{x_{i+1}} \left[ \frac{\partial^m \hat{\mu}_i(p, x)}{\partial x^m} \right]^2 dx$ .

8. 
$$\frac{\partial^{m} \hat{\mu_{i}}(p,x)}{\partial x^{m}} : \frac{\partial^{m} \hat{\mu_{i}}(p,x)}{\partial x^{m}} = \frac{\partial^{m}}{\partial x^{m}} \left[ \sum_{j=0}^{p} \alpha_{ij} x^{j} \right] = \frac{\partial^{m}}{\partial x^{m}} \left[ \sum_{j=m}^{p} \alpha_{ij} x^{j} \right] = \sum_{j=m}^{p} \frac{j!}{(j-m)!} \alpha_{ij} x^{j-m}.$$

9.  $\Lambda_i(k,m,p)$ :

$$\Lambda_{i}(k, m, p) = \int_{x_{1}}^{x_{i+1}} \left[ \sum_{j=m}^{p} \frac{j!}{(j-m)!} \alpha_{ij} x^{j-m} \right]^{2} dx = \sum_{j=m}^{p} \sum_{l=m}^{p} \left\{ \frac{j!}{(j-m)!} \frac{l!}{(l-m)!} \alpha_{ij} \alpha_{il} \left[ \frac{x_{i+1}^{j+l-2m+1} - x_{i}^{j+l-2m+1}}{j+l-2m+1} \right] \right\}$$

.

10. Minimization of 
$$\Lambda_i(k, m, p)$$
:  $\frac{\partial \Lambda_i(k, m, p)}{\partial \alpha_{ij}} = 0 \Rightarrow 2\overline{\alpha_{iq}}\beta_{qq} + \sum_{j=m, j\neq q}^p \alpha_{ij}\beta_{qj} = 0,$ 

$$m \leq j \leq p.$$

- Here  $\beta_{qj} = \frac{q!}{(q-m)!} \frac{j!}{(j-m)!} \left\{ \frac{x_{i+1}^{q+j-2m+1} x_i^{q+j-2m+1}}{q+j-2m+1} \right\}.$
- $\bullet \quad \overline{\alpha_{iq}} = -\frac{1}{\beta_{aa}} \sum_{l=m,l\neq a}^{p} \alpha_{il} \beta_{ql} .$
- Since  $\frac{\partial^2 \Lambda_i(k, m, p)}{\partial \alpha_{ij}^2} = \beta_{qq}$  and  $\beta_{qq} > 0$ ,  $\overline{\alpha_{iq}}$  corresponds to the minimum of  $\Lambda_i(k, m, p)$ .
- Thus, if  $x_i = 0$  and  $x_{i+1} = 1$ ,  $\beta_{qj}$  becomes  $\beta_{qj} = \frac{q!}{(q-m)!} \frac{j!}{(j-m)!} \left\{ \frac{1}{q+j-2m+1} \right\}$

.

# 11. <u>Polynomial v Splines – Number of unknowns</u>:

- Number of coefficients (unknown) => p+1
- Number of Nodal Start/End Values (known) => 2
- Number of Calibrated coefficients from the  $C^k$  criterion (known): k

- Net number of unknowns: p+1-2-k=p-k-1.
- 12. Ordered Unknown Coefficient Set in Polynomial  $\underline{v}$  Splines: Given that  $y_i = \sum_{j=0}^{p} \alpha_{ij} x^j$ ,  $\alpha_{i0}$  through  $\alpha_{ik}$ , as well as  $\alpha_{ip}$ , are known.
  - $\alpha_{iq}$  where  $k+1 \le q < p$  are the unknown coefficients.
  - For e.g., for  $C^1$  cubic polynomial spline, the number of unknowns are p-k-1=3-1-1=1.
- 13. <u>Maximum number of equations available from Optimizing  $\nu$  Splines:</u> Number of equations available from the optimization is p-1-m+1=p-m.
  - Determinacy criterion => Thus if p-m < p-k-1, or m > k+1, there are no solutions!
  - Alternatively, for completeness, derive m from k as m = k + 1 for completeness.
  - Finally, if  $k_{input} < p-2$ , optimizing run is needed.
- 14. <u>Advantage of Basis Curve Optimizing Formulation</u>: This formulation can readily/easily incorporate linearized constraints in an automatic manner as long as the explicit constraints are re-cast to be specified with the current segment.

# **Alternate Tension Spline Formulations**

1. <u>Kaklis-Pandelis Tension Spline</u>: As described in Kaklis and Pandelis (1990), here  $f(t) = f(x_i)[1-t] + f(x_{i+1})t + c_it[1-t]^{m_i} + d_it^{m_i}[1-t], \text{ where } t = \frac{x-x_i}{x_{i+1}-x_i}, \text{ and } m_i \text{ is the } t = \frac{x-x_i}{x_{i+1}-x_i}$ 

Kaklis-Pandelis shape-controlling tension polynomial exponent.

- $m_i = 2$  corresponds to the cubic spline interpolant on  $[x_i, x_{i+1}]$ .
- $m_i \to \infty$  corresponds to linear interpolant on  $[x_i, x_{i+1}]$ .
- 2. <u>Manni's Tension Spline</u>: The methodology is explained in detail in Manni (1996a), Manni and Sablionniere (1997), and Manni and Sampoli (1998). Here,

 $f_i(x) = p_i [q_i^{-1}(x)]$  on  $[x_i, x_{i+1}]$  where  $p_i$  and  $q_i$  are cubic polynomials. Further,  $q_i$  is strictly increasing in  $[x_i, x_{i+1}]$ , so that  $q_i^{-1}$  is well defined (Manni (1996b)).

- The boundary conditions are:  $f_i'(x_i) = d_i$ ; further, we impose that  $p_i'(x_i) = \lambda_i d_i$ ,  $q_i'(x) = \lambda_i$ ,  $p_i'(x_{i+1}) = \mu_i d_{i+1}$ , and  $q_i'(x_{i+1}) = \mu_i$  (see Manni (2001)). The claim is that if  $\lambda_i = \mu_i = 1$ ,  $q_i(x) = x$ , thus  $f_i$  becomes cubic. Also if  $\lambda_i = \mu_i = 0$ ,  $f_i$  reduces to linear.
- 3. KLK Splines: Next section is completely devoted to this.

# **Koch-Lyche-Kvasov Tension Splines**

### Introduction

- 1. Exponential B-Spline Specification: Expounded in detail in Cline (1974), Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000). First extend the knot set with 6 new points  $t_{-2}$ ,  $t_{-1}$ ,  $t_0$ ,  $t_{M+1}$ ,  $t_{M+2}$ , and  $t_{M+3}$  such that  $t_{-2} < t_{-1} < t_0 < t_1$  and  $t_M < t_{M+1} < t_{M+2} < t_{M+3}$ , but arbitrary otherwise.
- 2. Exponential Hat Functions:
  - $B_{i,2}(t) = \psi''(t)$  for  $t_i \le t \le t_{i+1}$ , and
  - $B_{j,2}(t) = \phi''(t)$  for  $t_{j+1} \le t \le t_{j+2}$ , where
  - $\psi_j(t) = \frac{\sinh[\sigma(t-t_j)] \sigma(t-t_j)}{\sigma^2 \sinh[\sigma(t_{j+1}-t_j)]}$ , and
- 3. Properties of the  $B_{j,k}(t)$  Splines:  $B_{j,2}(t)$  as defined above is the basis on top of which all the higher order splines are built.  $B_{j,2}(t)$  is non-zero only for  $t \in [t_j, t_{j+2}]$ , where  $j \in [-1,0,...,M]$ .
- 4. <u>Layout of Base Monic Setup</u>: With reference to figure 9, the monic basis function  $B_{j,2}$  may be estimated from the corresponding primitive hat functions  $\psi$  and  $\phi$  (referred to as A and B respectively in Figure 9) as:
  - $B_{j,2} = \psi_j''(t)$  for  $t_j \le t < t_{j+1}$ .
  - $B_{j,2} = \phi_{j+1}$ "(t) for  $t_{j+1} \le t < t_{j+2}$ .
  - $B_{i,2} = 0$  otherwise.
- 5. <u>Monic B-Spline Normalizer</u>:

• 
$$C_{j,2} = \int_{t_j}^{t_{j+2}} B_{j,2}(y) dy = \int_{t_j}^{t_{j+1}} \psi_j''(y) dy + \int_{t_{j+1}}^{t_{j+2}} \phi_j''(y) dy$$

• 
$$C_{j,2} = \psi_j'(t_{j+1}) - \psi_j'(t_j) + \phi_{j+1}'(t_{j+2}) - \phi_{j+1}'(t_{j+1})$$

• 
$$C_{j+1,2} = \psi_{j+1}'(t_{j+2}) - \psi_{j+1}'(t_{j+1}) + \phi_{j+2}'(t_{j+3}) - \phi_{j+2}'(t_{j+2})$$

6. Monic B-Spline Cumulative Normalized Integrand:

• 
$$\Lambda_{i,2} = 0$$
 for  $t < t_i$ .

$$\bullet \quad \Lambda_{j,2} = 1 \text{ for } t \ge t_{j+2}.$$

7. Monic B-Spline Scaled Integrand:

• 
$$\Lambda_{j,2} = 0$$
 for  $t < t_j$ .

• 
$$\Lambda_{j,2} = \frac{\psi_j'(t) - \psi_j'(t_j)}{\psi_j'(t_{j+1}) - \psi_j'(t_j) + \phi_{j+1}'(t_{j+2}) - \phi_{j+1}'(t_{j+1})}$$
 for  $t_j \le t < t_{j+1}$ .

• 
$$\Lambda_{j,2} = \frac{\psi_{j}'(t_{j+1}) - \psi_{j}'(t_{j}) + \phi_{j+1}'(t) - \phi_{j+1}'(t_{j+1})}{\psi_{j}'(t_{j+1}) - \psi_{j}'(t_{j}) + \phi_{j+1}'(t_{j+2}) - \phi_{j+1}'(t_{j+1})} \text{ for } t_{j+1} \leq t < t_{j+2}.$$

• 
$$\Lambda_{j,2} = 1$$
 for  $t \ge t_{j+2}$ .

8. Monic B-Spline Scaled Integrand:

$$B_{j,3}(t) = \Lambda_{j,2}(t) - \Lambda_{j+1,2}(t) = \int_{t_{j}}^{t} B_{j,2}(y) dy - \int_{t_{j+1}}^{t} B_{j+1,2}(y) dy - \int_{t_{j+1}}^{t} B_{j+1,2}(y) dy - \int_{t_{j+1}}^{t} B_{j+1,2}(y) dy = \int_{t_{j+1}}^{t} B_{j+1,2}(y) dy$$

9. Quadratic and Cubic Exponential Tension Splines: Higher order splines are recursively defined from  $B_{j,k}(t) = \Lambda_{j,k-1}(t) - \Lambda_{j+1,k-1}(t)$  where:

• 
$$\Lambda_{j,k}(t) = 0$$
 for  $t \le t_j$ 

• 
$$\Lambda_{j,k}(t) = \frac{1}{\Omega_{j,k}} \int_{t_j}^t B_{j,k}(y) dy$$
 for  $t_j \le t \le t_{j+k}$ 

•  $\Lambda_{i,k}(t) = 1$  otherwise

Here  $\Omega_{j,k} = \int_{t_j}^{t_{j+k}} B_{j,k}(y) dy$ . Further, k = 2 and k = 3 correspond to quadratic and cubic

tension splines, respectively.

- 10. <u>Similarities between Exponential Tension B-Splines and Polynomial B-Splines</u>:

  Notice the similarities, the iterative higher-order definitions, and the partition of unity as well.
- 11. <u>Cubic Exponential Tension B-Spline</u>: This corresponds to the  $B_{j,k=4}(t)$  case, i.e.,

$$g(t) = \sum_{k=j-1}^{j+2} \beta_k B_{k-2,4}(t)$$
, with validity in the interval  $t \in [t_j, t_{j+4}]$ .

 Explicit Cubic Basis Representation => Using Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000), define:

$$\circ \quad z_j = \psi_{j-1}(t_j) - \phi_j(t_j)$$

$$\circ z_{j}' = \psi_{j-1}'(t_{j}) - \phi_{j}'(t_{j})$$
, and

$$\circ \quad y_j = t_j - \frac{z_j}{z_i}$$

$$o \quad b_{j,(1)} = \frac{b_{j+2} - b_{j+1}}{y_{j+2} - y_{j+1}}$$

$$o \quad b_{j,(2)} = \frac{b_{j,(1)} - b_{j,(-1)}}{z_{j+1}}$$

• Expanded g(t) in the new basis representation => For  $t \in [t_j, t_{j+4}]$ ,

$$g(t) = \sum_{k=j-1}^{j+2} \beta_k B_{k-2,4}(t) = \beta_j + \beta_{j-1,(1)} \{t - y_j\} + \beta_{j-1,(2)} \phi_j(t) + \beta_{j,(2)} \psi_j(t).$$
 This clearly

shows the similarity to the generalized Kaklis-Pandelis tension spline formulation. Retaining  $\phi_j(t)$  and  $\psi_j(t)$  this way helps generalize to other basis tension splines.

• Expansion of g(t) in basis function terms =>

$$g(t) = \beta_{j-1}\alpha_{j-1}(t) + \beta_{j}\alpha_{j}(t) + \beta_{j+1}\alpha_{j+1}(t) + \beta_{j+2}\alpha_{j+2}(t) \text{ where}$$

$$\alpha_{j-1}(t) = \frac{\phi_{j}(t)/z_{j}'}{y_{j} - y_{j-1}}$$

$$\alpha_{j}(t) = 1 - \frac{t - y_{j} + \phi_{j}(t)/z_{j}'}{y_{j+1} - y_{j}} - \frac{\phi_{j}(t)/z_{j}'}{y_{j} - y_{j-1}} + \frac{\psi_{j}(t)/z_{j}'}{y_{j+1} - y_{j}}$$

$$\alpha_{j+1}(t) = \frac{t - y_{j} + \phi_{j}(t)/z_{j}'}{y_{j+1} - y_{j}} - \frac{\psi_{j}(t)/z_{j+1}'}{y_{j+2} - y_{j-1}} + \frac{\psi_{j}(t)/z_{j+1}'}{y_{j+1} - y_{j}}$$

$$\alpha_{j+2}(t) = \frac{\psi_{j}(t)/z_{j+1}'}{y_{j+2} - y_{j+1}}$$

- Robust/Efficient Calculation of Hyperbolics => Renka (1987) and Rentrop (1980) outline some effective methods for this. For small  $\sigma$ , truncated Taylor series is accurate enough.
- 12. Piecewise Cubic Interpolant Expansion: Remember that, no matter what the basis tension functions are, for piecewise tension  $C^2$  continuity, they are expected to satisfy

$$d_{j} = \frac{\partial^{2} g(t)}{\partial t^{2}} - \sigma^{2} g(t) = \frac{t_{j+1} - t}{t_{j+1} - t_{j}} \left[ \left| \frac{\partial^{2} g(t)}{\partial t^{2}} \right|_{t=t_{j}} - \sigma^{2} g(t_{j}) \right] + \frac{t - t_{j}}{t_{j+1} - t_{j}} \left[ \left| \frac{\partial^{2} g(t)}{\partial t^{2}} \right|_{t=t_{j+1}} - \sigma^{2} g(t_{j+1}) \right]$$

for  $t \in [t_j, t_{j+1}]$ , i.e., this entity varies linearly across the segment.

• This may be re-cast as  $d_j = \beta_{j-1} \varpi_{j-1} + \beta_j \varpi_j + \beta_{j+1} \varpi_{j+1}$  where

$$\boldsymbol{\varpi}_{j-1} = \frac{\{1 - \sigma^2 \phi_j(t_j)\}/z_j'}{y_j - y_{j-1}} \quad \boldsymbol{\varpi}_{j+1} = \frac{\{1 - \sigma^2 \psi_{j-1}(t_j)\}/z_j'}{y_{j+1} - y_j}$$

$$\varpi_{j} = \beta_{j} \left[ 1 - \frac{\left\{ 1 - \sigma^{2} \phi_{j} \left( t_{j} \right) \right\} / z_{j}'}{y_{j} - y_{j-1}} - \frac{\left\{ 1 - \sigma^{2} \psi_{j-1} \left( t_{j} \right) \right\} / z_{j}'}{y_{j+1} - y_{j}} \right]$$

13. <u>Tension Spline Curvature Penalizing Norm</u>: The pure curvature penalizer may now be altered to become a curvature + length penalizer. Thus,

$$P_{Curv} = \lambda \int_{t_1}^{t_M} [\{y''(t)\}^2 + \sigma^2 \{y'(t)\}^2] dt. \text{ Notice that both } \{y''(t)\}^2 \text{ and } \sigma^2 \{y'(t)\}^2 \text{ (i.e., }$$

separated squares) are included individually in the set up.

- Simplification of the curvature penalty norm term for the Tension Splines =>  $P_{Curv} = \lambda \int_{t_1}^{t_M} \left[ \{y''(t)\}^2 + \sigma^2 \{y'(t)\}^2 \right] dt = g_{j+1}'' g_{j+1}' g_{j}'' g_{j}' d_{j} \left[ g_{j+1} g_{j} \right]. \text{ A simple}$  proof of this using integration by parts is available in Andersen (2005).
- Penalizing the segment length in addition to the segment curvature is valid for all spline formulations, of course. However, they may not be reducible/simplifiable as much as they are in tension splines.
- 14. Constrained Optimizer Estimate for  $\underline{\lambda}$ : If the RMS best-fit error is to be limited to  $\gamma^2$  where  $\gamma^2$  is an extraneously specified closeness of fit metric, the constraint may be expressed as  $\frac{1}{N} [\vec{V} c\vec{P}]^T W^T W [\vec{V} c\vec{P}] \leq \gamma^2$ .
  - Now the optimization minimizer attains contributions from best-fit, curvature penalty, and segment length penalties.
  - Step #1: For a given initial guess of  $\lambda$ , find the optimal co-efficient set  $\{\beta_i\}_{i=0}^{n-1}$ .
  - Step #2: Compute  $S(\lambda) = [BestFit]^2$ . If  $S(\lambda)$ , you are done. Otherwise use a suitable root finder to extract  $\lambda$ .
  - Step #3: The best-fit optimizer precision norm  $S(\lambda)$  is a declining function of  $\lambda$ . If a root exists, the root finder procedure should be able to find it.
  - λ estimation in the context of curve building is treated in Tanggaard (1997)
     (using the GCV technique of Craven and Wahba (1979)) and Andersen (2005).
- 15. <u>Drawbacks of the above method</u>: This involves yet another non-linear root extractor. Other non-linear root extraction parts in curve building are:
  - Non-linear boot-strapping
  - Non-linear boundary condition in spline calibration.
     Thus, the stability of the precision norm technique outlined above is riddled with challenges.
- 16. <u>Parallel with Hagan-West Forward Interpolator</u>: In Hagan-West (Hagan and West (2006)) minimalist quadratic interpolator, the segment length is incorporated in a

- slightly different way as a minimizer of the k+1 jumps at the knots (i.e., if  $C^2$ , minimizing  $C^3$  at the knots).
- 17. The other Tension Splines: They all have the property that the tension parameter moves smoothly from cubic (low tension) to linear (high tension), and have different forms for  $\phi$  and  $\psi$ . These forms may make them computationally less expensive too.
  - Non-uniform Rational Cubic Tension Spline with linear Denominator =>

$$\Psi_{j} = \frac{(t - t_{j})^{3}}{(t_{j+1} - t_{j})[1 + \sigma_{j}(t_{j+1} - t)][6 + 6\sigma_{j}(t_{j+1} - t_{j}) + 2\sigma_{j}(t_{j+1} - t_{j})^{2}]}$$

$$\phi_{j} = \frac{\left(t_{j+1} - t\right)^{3}}{\left(t_{j+1} - t_{j}\right)\left[1 + \sigma_{j}\left(t - t_{j}\right)\right]\left[6 + 6\sigma_{j}\left(t_{j+1} - t_{j}\right) + 2\sigma_{j}\left(t_{j+1} - t_{j}\right)^{2}\right]}$$

Non-uniform Rational Cubic Tension Spline with Quadratic Denominator =>

$$\Psi_{j} = \frac{(t - t_{j})^{3}}{[(t_{j+1} - t_{j}) + \sigma_{j}(t - t_{j})(t_{j+1} - t)][6 + 6\sigma_{j}(t_{j+1} - t_{j}) + 2\sigma_{j}(t_{j+1} - t_{j})^{2}]}$$

Non-uniform Exponential Rational Spline =>

$$\Psi_{j} = \frac{(t - t_{j})^{3} \exp[-\sigma_{j}(t_{j+1} - t)]}{(t_{j+1} - t_{j})[6 + 6\sigma_{j}(t_{j+1} - t_{j}) + 2\sigma_{j}(t_{j+1} - t_{j})^{2}]}$$

$$\phi_{j} = \frac{(t_{j+1} - t)^{3} \exp[-\sigma_{j}(t - t_{j})]}{(t_{j+1} - t_{j})[6 + 6\sigma_{j}(t_{j+1} - t_{j}) + 2\sigma_{j}(t_{j+1} - t_{j})^{2}]}$$

18. Tension Implied by the Basis Function Set: Given the tension  $C^2$  interpolant relation

$$\frac{\partial f}{\partial x} + \sigma_j^2 \frac{\partial^3 f}{\partial x^3} = Cons \tan t$$
 inside a given segment j, we can infer  $\sigma_j$  from

$$\sigma_{j} = -\frac{\left|\frac{\partial f}{\partial x}\right|_{x=1} - \left|\frac{\partial f}{\partial x}\right|_{x=0}}{\left|\frac{\partial^{3} f}{\partial x^{3}}\right|_{x=1} - \left|\frac{\partial^{3} f}{\partial x^{3}}\right|_{x=0}}.$$

19. <u>Caveat for using KLK-type Splines for Local State Shape Proxying</u>: Often (and this may be true for other B Splines as a whole too), the B Spline basis choice may

produce segment node edge values and their corresponding derivatives of zero. In this case, you may have a singular calibration matrix that does not calibrate. In particular, this is the case for iterated B Splines that are constructed to vanish and fade rapidly at the edges. This poses for problems for segment-local splines (that may span between 0 and 1 within a given segment).

• How does the KLK formulation avoid this? It is because it is built off of a cubic B Spline, thus works primarily for that case. KLK retains the basis representation out from a workable/calibratable raw cubic B Spline form that is set to be "well-behaved" at the edges (by definition) at the cubic basis level. The B Splines that follow the typical iterative generation formulation end up "destroying the raw basis construction information" if set up from above (i.e.,  $\psi$  above the cubic level becomes  $\psi$ " at the lowest hat level).

# **Smoothing Splines**

## **Penalty Minimization Risk Function**

- 1. <u>Penalty Minimizer Estimator Metric</u>: Choice of the "normalized curvature area" shown in figures 5) and 6) are two possible penalty estimator choices. Obviously, closer the area is to zero, the better the penalizing match is.
- 2. <u>Dimensionless Penalizing Fit Metric</u>: Choosing the representation in 5), and recognizing that the segment is set in the flat base (0,1), we can derive the representation in 7).
- 3. Dimensionless Penalty Estimator (DPE): Using Figure 7), we now define DPE as

$$DPE = \frac{Area_{ShadedPart}}{Area_{ABCD}} = \frac{\int_{x_i}^{x_{i+1}} \left[ \frac{\partial^m \hat{\mu}(x)}{\partial x^m} \right]^2 dx}{\max \left\{ \left[ \frac{\partial^m \hat{\mu}(x)}{\partial x^m} \right]^2 \right\} (x_{i+1} - x_i)}$$

- 4. <u>Pros/Cons of the above Representation of DPE</u>: If the basis functions have near-delta functional forms (Figure 8), DPE will still remain ≈ 0, and the metric is not very meaningful in that case. Fortunately, such delta-type basis functions are rare.
- 5. <u>Aggregate DPE Measure</u>: Need a consolidated DPE metric that spans across all the segments in a span, i.e., the span DPE.

# **Smoothing Splines Setup**

- 1. <u>Process Control using Weights</u>: Dimensionless units (such as Reynolds' number) can effectively account for the ratio of competing natural forces. Similar use can be done for process control to be able to guide/control between 2 or more competing objectives. For example in the instance of the smoothing spline:
  - First Objective => Closeness of match using the most faithful reproducer, or curve fit.

- Second Objective => Smoothest curve through the given points, without necessarily fitting them of course, "smoothest" possible "curve" is a straight line.
- Penalizing Smootheners: Penalizing smootheners are the consequence of Bayes
  estimation applied on the Quadratic Penalties with Gaussian Priors (also referred to with
  maxim "The Penalty is the Prior").
- 3. Smoothing Spline Formulation: Given  $x_1 < x_2 < ... < x_n$ , and the function  $\mu$  that fits the points  $[x_i, Y_i]$  from  $Y_i = \mu(x_i)$  (see Hastie and Tibshirani (1990) and Smoothing Spline (Wiki)). The smoothing spline estimate  $\hat{\mu}$  is the minimizer

$$\min \arg \left\{ \Lambda \left( \hat{\mu}, \lambda \right) = \frac{1}{n} \sum_{i=1}^{1} \left[ Y_i - \hat{\mu}(x_i) \right]^2 + \lambda \int_{x_1}^{x_n} \left[ \frac{\partial^k \hat{\mu}(x)}{\partial x^k} \right] dx \right\}$$

- $\Lambda(\hat{\mu}, \lambda)$  is the **Spline Objective Function**.
- $\frac{1}{n}$  is needed to the left term to make it finite as  $n \to \infty$ , otherwise  $\lambda$  will also have to be infinite.
- The derivative "k" corresponds to what makes  $\left[\frac{\partial^k \hat{\mu}(x)}{\partial x^k}\right]$  linear. Thus, for cubic splines, k = 2.
- 4. <u>Bias Curvature/Variance Fit Trade-off</u>: Smaller the  $\lambda$ , the more you will fit for bias (low curvature penalty). Bigger the  $\lambda$ , more you fit for curvature/roughness penalty.
- 5. <u>Curvature Penalty Minimizer Spline</u>: It can be theoretically shown that the curvature penalty minimizer spline is a cubic spline. Here is how.
  - First, notice that any spline of degree  $\geq$  0 can reproduce the knot inputs.
  - By default, curvature corresponds to k = 2. Thus,  $\left[\frac{\partial^2 \hat{\mu}(x)}{\partial x^2}\right]$  varies linearly inside a segment, thus this becomes the least possible curvature.
  - Higher order splines will have a non-linear curvature.
  - Lesser order (spline order less than 3) will violate the C<sup>2</sup> continuity constraint.

- 6. <u>Bias Curvature/Variance Fit Trade-off</u>: Smaller the  $\lambda$ , the more you will fit for bias (low curvature penalty). Bigger the  $\lambda$ , more you fit for curvature/roughness penalty.
- 7. <u>Smoothing Output Criterion</u>:
  - Speed of Fitting
  - Speed of Optimization
  - Boundary Effects
  - Sparse, Computationally Efficient Designs
  - Semi-Parametric Models
  - Non-normal Data
  - Ease of Implementation
  - Parametrically determinable Limits
  - Specialized Limits
  - Variance Alteration/inflation
  - Adaptive Flexibility Possible
  - Adaptive Flexibility Available
  - Compactness of Results
  - Conservation of data distribution moments
  - Easy Standard Errors
- 8. Smoothing vs. Over-fitting: Since  $\lambda$  is a control parameter, it can always be attained by a parametric specification. To estimate optimal value of  $\lambda$  against over-fitting, use one of the following other additional criteria to penalize the extra parameters used in the fit, such as the following. Each one of them comes with its own advantages/disadvantages.
  - Cross-validation
  - Global Cross-Validation
  - Akaike Information Criterion
  - Bayesian Information Criterion
  - Deviance
  - Kullback-Leibler Divergence metric
- 9. Segment Stiffness Control:  $\lambda$  may also be customized to behave as a segment stiffener or a penalty/stiffness controller, thus providing extra knobs for the optimization control.

## 10. Relation of Lagrangian to Smoothing Spline:

- Lagrangian objective function is used to optimize a multi-variate function L(x, y) to incorporate the constraint g(x, y) = c as  $\Lambda(x, y, z) = L(x, y) + \lambda[g(x, y) c]$ . Here  $\lambda$  is the Lagrange multiplier.
- Optimized formulation of the smoothing spline is given by minimizing the spline objective function (a form of optimization)

$$\Lambda\left(\hat{\mu},\lambda\right) = \frac{1}{n} \sum_{i=1}^{1} \left[ Y_i - \hat{\mu}(x_i) \right]^2 + \lambda \int_{x_i}^{x_n} \left[ \frac{\partial^k \hat{\mu}(x)}{\partial x^k} \right] dx. \text{ Here } \lambda \text{ is the spline objective}$$

function shadow price of curvature penalty, i.e.,  $\frac{\partial \Lambda\left(\hat{\mu},\lambda\right)}{\partial c} = -\lambda$ , where c is the constraint constant defined analogous to the constraint constant in the Lagrangian objective function:  $\int_{x_1}^{x_n} \left[ \frac{\partial^k \hat{\mu}(x)}{\partial x^k} \right] dx = c$ .

# **Ensemble Averaging vs. Basis Spline Representation**

- 1. Parallel between Spline Representation and Ensemble Averaging Techniques: From a real-valued inference (i.e., regression + transformed classification) point-of-view, there are significant similarities between ensemble averaging techniques and basis spline representation techniques. While ensemble averaging attempts to aggregate over hypotheses set, multi-spline basis representation attempts to represent the splines over the set of the basis spline representation function set. Further, there are also parallels in the way in which the weights are inferred; for basis splines, this is achieved by a combination of best-fit and penalization, whereas for the ensemble aggregator this done via the variance-bias optimization mechanism.
- 2. <u>Difference</u>: Ensemble averaging may be viewed as a dual pass training exercise effectively the first training pass trains the individual response basis functions themselves, and the second pass trains the weights across the basis function set.

- 3. <u>Focus of the Training Passes</u>: Focus of the first pass in ensemble averaging is simply bias reduction, i.e., enhancing the closeness of fit and reduction of Bayes' risk. The second pass performs the ensemble averaging with a view to reducing the variance this is comparable to the smoothening pass.
- 4. <u>Ensemble Averaging vs. Multi-Pass State Inference</u>: Boas reduction is comparable to the shape preservation pass, whereas the ensemble averaging/variance reduction is comparable to the smoothening pass.

## 5. <u>Differences between Ensemble Averaging and Multi-Pass State Inference</u>:

- a. The shape preserving pass ends up emitting a sequence of parameters that correspond to the stretches across the univariate predictor ranges to represent a SINGLE latent state.
- b. The calibration run during the shape preserving pass produces a set of calibrated parameters for the full set of basis splines for shape preservation (i.e., error minimization).
- c. Training each basis function separately druing the bias reduction phase of ensemble averaging does not really purport to "infer" any latent state.
- d. The second phase of ensemble aggregation simply re-works the basis weights across all the "low bias" basis functions, again no notion of "re-inferrring of states" involved.
- e. The smoothing phase of the multi-phase latent-state construction may work on a latent state quantification metric that is different from the shape preserving pass; while this does loosen the shape preservation impact, it is no more different to the equivalent step in ensemble averaging.

# **Least Squares Best Fit + Curvature + Segment Length Penalty Formulation**

#### 1. Nomenclature:

•  $p = 0,...,q-1 \Rightarrow$  Points to Fit for the Least Squares Penalty

- i = 0,...,n-1 => The Basis Functions Index
- j = 0,...,m-1 =>Number of Ordinate Points
- $r \Rightarrow$  Curvature Penalizer Derivative
- s => Length Penalizer Derivative
- $k \Rightarrow k$ -Separation to be achieved during the Formulative Derivation

2. The Formulation: 
$$P = \sum_{p=0}^{q-1} [\hat{y}_p - y_p]^2 + \lambda \int_{x_0}^{x_m} \left\{ \left( \frac{\partial^r \hat{y}}{\partial x^r} \right)^2 + \sigma^2 \left( \frac{\partial^s \hat{y}}{\partial x^s} \right)^2 \right\} dx \text{ where}$$

$$\hat{y}(x) = \sum_{i=0}^{n-1} \beta_i f_i(x).$$

- 3. <u>Segment-Level Decomposition</u>: Segment-level decomposition ensures optimal segment coefficient formulation to within the boundaries of a segment (from the least squares fit point of view) however, not necessarily global optimum. Further, these optimal constraints provide an extra degree of freedom at the segment level, and not necessarily at the stretch/span level.
- 4. Segment-Level Decomposition Formulation:

$$\mathbf{P} = \sum_{p=0}^{q-1} \left[ \hat{y}_p - y_p \right]^2 + \lambda \int_{x_{j-1}}^{x_j} \left\{ \left( \frac{\partial^r \hat{y}}{\partial x^r} \right)^2 + \sigma_j^2 \left( \frac{\partial^s \hat{y}}{\partial x^s} \right)^2 \right\} dx = \sum_{p=0}^{q-1} \mathbf{M}_p + \lambda \left[ \mathbf{X}_j + \sigma_j^2 \Lambda_j \right] \text{ where}$$

$$\mathbf{M}_P = \left[ \hat{y}_p - y_p \right]^2, \ \mathbf{X}_j = \int_{x_{j-1}}^{x_j} \left( \frac{\partial^r \hat{y}}{\partial x^r} \right)^2 dx, \text{ and } \Lambda_j = \int_{x_{j-1}}^{x_j} \left( \frac{\partial^s \hat{y}}{\partial x^s} \right)^2 dx.$$

5. <u>Least Squares Minimization Review</u>: From earlier,

• 
$$\mathbf{M}_{P} = [\hat{y}_{p} - y_{p}]^{2} = \left[\sum_{i=0}^{n-1} \beta_{i} f_{i}(x_{p}) - y_{p}\right]^{2}.$$

$$\bullet \quad \frac{\partial \mathbf{M}_{P}}{\partial \beta_{k}} = 2f_{k}\left(x_{p} \left[\sum_{i=0}^{n-1} \beta_{i} f_{i}(x_{p}) - y_{p}\right] = 0 \Rightarrow \sum_{i=0}^{n-1} \beta_{i} f_{i}(x_{p}) - y_{p} = 0.$$

- $\frac{\partial^2 \mathbf{M}_P}{\partial \beta_k^2} = 2f_k^2(x_p) \ge 0$ . Therefore a minimum exists.
- 6. Curvature Penalty Minimization: Again, from earlier,

• 
$$X_j = \int_{x_{i-1}}^{x_j} \left( \frac{\partial^r \hat{y}}{\partial x^r} \right)^2 dx = \int_{x_{i-1}}^{x_j} \sum_{i=0}^{n-1} \left( \beta_i \frac{\partial^r f_i(x)}{\partial x^r} \right)^2 dx$$
.

$$\frac{\partial X_{j}}{\partial \beta_{k}} = 2 \sum_{i=0}^{n-1} \beta_{i} \int_{x_{j-1}}^{x_{j}} \left( \frac{\partial^{r} f_{k}(x)}{\partial x^{r}} \right) \left( \frac{\partial^{r} f_{i}(x)}{\partial x^{r}} \right) dx = 0 \Rightarrow \sum_{i=0}^{n-1} \beta_{i} \int_{x_{j-1}}^{x_{j}} \left( \frac{\partial^{r} f_{k}(x)}{\partial x^{r}} \right) \left( \frac{\partial^{r} f_{i}(x)}{\partial x^{r}} \right) dx = 0$$
for each  $k$ .

- Further,  $\frac{\partial^2 \mathbf{X}_j}{\partial \beta_k^2} = 2\beta_i \int_{x_{i-1}}^{x_j} \left( \frac{\partial^r f_k(\mathbf{x})}{\partial \mathbf{x}^r} \right)^2 d\mathbf{x} \ge 0$  for  $x_j > x_{j-1}$ , thus a minimum exists.
- 7. Segment Length Penalty Minimization: Similar to the curvature penalty, we get,

$$\bullet \quad \Lambda_{j} = \int_{x_{j-1}}^{x_{j}} \left( \frac{\partial^{s} \hat{y}}{\partial x^{s}} \right)^{2} dx = \int_{x_{j-1}}^{x_{j}} \sum_{i=0}^{n-1} \left( \beta_{i} \frac{\partial^{s} f_{i}(x)}{\partial x^{s}} \right)^{2} dx.$$

- $\frac{\partial \Lambda_j}{\partial \beta_k} = 0 \Rightarrow \sum_{i=0}^{n-1} \beta_i \int_{x_{i-1}}^{x_j} \left( \frac{\partial^s f_k(x)}{\partial x^s} \right) \left( \frac{\partial^s f_i(x)}{\partial x^s} \right) dx = 0$  for each k.
- Finally,  $\frac{\partial^2 \Lambda_j}{\partial \beta_k^2} = 2\beta_i \int_{x_{j-1}}^{x_j} \left( \frac{\partial^s f_k(x)}{\partial x^s} \right)^2 dx \ge 0$  for  $x_j > x_{j-1}$ , thus a minimum exists.
- 8. Combining it all:

$$\sum_{i=0}^{n-1} \beta_i \left\{ f_i(x_p) + \lambda \int_{x_{j-1}}^{x_j} \left( \frac{\partial^r f_k(x)}{\partial x^r} \right) \left( \frac{\partial^r f_i(x)}{\partial x^r} \right) dx + \lambda \sigma_j^2 \int_{x_{j-1}}^{x_j} \left( \frac{\partial^s f_k(x)}{\partial x^s} \right) \left( \frac{\partial^s f_i(x)}{\partial x^s} \right) dx \right\} = y_p.$$

## **Alternate Smootheners**

- 1. Compendium of Smoothing Methods:
  - Kernel Smoothing with or without binning.
  - Local Regression with or without binning.
  - Smoothing Splines with or without band solvers.
  - Regression splines with fixed/adaptive knots.
  - Penalizing B Splines.
  - Density Smoothing.
- 2. <u>Kernel Bandwidth Selector</u>: Kernel bandwidth selection is analogous to the optimal knot point selection employed in the regression spline schemes.

- Remember that the kernel methods essentially use the periodic functions as their basis functions.
- 3. <u>Regression Splines</u>: Here the data is simply fit to a (hugely) reduced set of basis spline functions, typically using least squares, without any smoothness penalty.
  - Penalized regression splines are pretty much the same as regression splines in that
    they do use a reduced set of basis splines. However, they do impose a roughness
    penalty. Penalized regression splines are also referred to as smoothing splines.
  - Polynomial Regression Splines do curve fitting/regression analysis using selective insertion/removal of knots. Knots are added according to the Rao criterion, and removed according to the Wald criterion.
    - Log Splines are a customization of the polynomial regression splines targeted for density estimation. The log of the density is modeled as a cubic spline.
  - Tension Regression Splines => In addition to the curvature penalty and the least squares fit penalty, tension regression splines also penalize the segment length.
- 4. <u>Base Density Smoothing Formulation</u>: Log-likelihood density smoothing is analogous to maximizing the multinomial likelihood histogram  $\log \left[ \prod_{i=1}^{m} p_i^{y_i} \right]$ , where  $y_i$  is the empirical observation count, and  $p_i$  is the probability of finding an observation in the cell i.

# **Multi-dimensional Splines**

- 2D Wire Span Surface Stretch: Here a 2D Surface is built off of discrete, separated
  univariate span chords called wires, and the inner nodes are splined in using a
  targeted "wiring" spline. While this is naturally less smooth compared to the 2D basis
  splines (and surface energy minimizing splines) below, it does provide targeted
  customization of particular chords.
- 2. Non-symmetrical multi-dimensional Variates: Again, considering 2D as an example, it makes sense to use the basis splines separately across both  $x_1, x_2$ , as in

$$\hat{\mu}(x_1, x_2) = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \beta_{ij} B_i(x_1) B_j(x_2).$$

- 3. <u>Bi-polynomial 2D Spline</u>: For the 2D Segment Range  $x \to [x_i, x_{i+1}]$  and  $y \to [y_i, y_{i+1}]$ , working in the local variate space  $t = \frac{x x_i}{x_{i+1} x_i}$  and  $u = \frac{y y_i}{y_{i+1} y_i}$ , we transform the spline basis on to the local representation basis as  $f_{i,j}(t,u) = \sum_{k=0}^{m} \sum_{l=0}^{n} \beta_{ij,kl} t^k u^l$ .
- 4. <u>Bi-linear 2D Spline</u>: This produces a  $C^0$  surface. Here k = l = 1, therefore the first derivatives (and on) are discontinuous on the grid boundaries. From the observation set  $\{z_{i,j}\}$ , we get from the boundary match the following values for  $\beta_{ij,kl}$ :
  - $\bullet \qquad \beta_{ij,00} = z_{i,j}$
  - $\beta_{ij,01} = -z_{i,j} + z_{i,j+1}$
  - $\bullet \qquad \beta_{ij,10} = -z_{i,j} + z_{i+1,j}$
  - $\bullet \qquad \beta_{ij,11} = z_{i,j} + z_{i+1,j+1} z_{i+1,j} z_{i,j+1}$
- 5. <u>Bi-Cubic Interpolation</u>: This produces a  $C^1$  surface. Here k = l = 3, therefore the first, second, and the first cross derivatives (i.e., f(x, y),  $\frac{\partial f(x, y)}{\partial x}$ ,  $\frac{\partial f(x, y)}{\partial y}$ ,

$$\frac{\partial^2 f(x,y)}{\partial x^2}$$
,  $\frac{\partial^2 f(x,y)}{\partial y^2}$ , and  $\frac{\partial^2 f(x,y)}{\partial x \partial y}$ ) are continuous across the grid boundaries.

From the observation set  $\{z_{i,j}\}$ , their first derivatives, and their cross derivatives, we get from the boundary match the following values for  $\beta_{ij,kl}$  as before. The common way is to cast these as a sequence of 2D relations by unraveling the continuity constraints, and thereby linearizing the formulation.

- Symmetrical Multi-dimensional variates: The trivial univariate ordering
   x<sub>1</sub> < x<sub>2</sub> < ... < x<sub>n</sub> needs revising in the context of certain multivariates, e.g.,
   symmetrical multivariates (Smith, Price, and Lowser (1974), Graham (1983), and Lee
   (1989)).
  - A general "distance from focal node"  $t_i$  makes to more sense to set in the ascending order. Thus  $t_i = \sqrt{(x_i x_F)^2 + ... + (z_i z_F)^2}$ , where  $[x_F,...,z_F]$  are the multivariate nodes corresponding to the focal node.
  - Alternatively, the distance from the prior node parametrizer  $t_i = \sqrt{(x_{i+1} x_i)^2 + ... + (z_{i+1} z_i)^2}$  may also work.
  - Use Cartesian/radial/axial basis functions to formulate the segments in terms of the surface vector coefficients in "symmetrical variate" situations.
- 7. <u>Surface Energy Minimization</u>: Surface energy minimization using the "sigma" tension parameter formulate equation.
  - Thin Plate Spline (Duchon (1976), Duchon (1977)): This is simply 2D spline interpolation, achieved by minimizing the surface bending energy, the minimization of  $E[f] = \int_{\mathbb{R}^2} |\nabla^2 f(x,y)|^2 dx dy$ , where

$$\left|\nabla^2 f(x,y)\right|^2 = \frac{\partial^2 f(x,y)}{\partial x^2} + \frac{\partial^2 f(x,y)}{\partial y^2} + \frac{\partial^2 f(x,y)}{\partial x \partial y}.$$

• Thin plate splines are an effective way to achieve surface energy minimization, i.e., for a 2D surface, the smoothing spline surface may be created by the minimization of the following least squares surface spline objective function

$$\Lambda\left(\hat{\mu}, x_{1}, x_{2}, \lambda\right) = \frac{1}{n} \sum_{i=1}^{1} \left[Y_{i} - \hat{\mu}(x_{1i}, x_{2i})\right]^{2} + \lambda \int_{x_{11}}^{x_{1n}} \int_{x_{21}}^{x_{2n}} \left[\left(\frac{\partial^{2} \hat{\mu}(x)}{\partial x_{1}^{2}}\right)^{2} + \left(\frac{\partial^{2} \hat{\mu}(x)}{\partial x_{1} \partial x_{2}}\right) + \left(\frac{\partial^{2} \hat{\mu}(x)}{\partial x_{2}^{2}}\right)^{2}\right] dx_{1} dx_{2}$$

- . Again, apparently this is more appropriate if  $x_1, x_2$  are symmetrical.
- 8. <u>Elastic Maps Method for Manifold Learning</u>: This method combines the least squared penalty for the approximation error with the bending/torsional-stretching penalty for the proxy manifold. It then uses a coarse discretization to extract the solution for the optimization problem.

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### **Spline Library Software Components**

Functionality behind Spline Library is available across 10 core functional packages, 2 samples package and 1 regression test package.

The core functional packages are:

- Univariate function package
- Univariate Calculus package
- Spline Parameters package
- Spline Basis Function Set package
- Spline Segment package
- Spline Stretch Package
- Spline Grid/Span Package
- Spline PCHIP Package
- B Spline Package
- Tension Spline Package

The sample functional packages are:

- Spline Sample package
- Stretch Sample package

### **Univariate Function Package (org.drip.quant.function1D)**

The univariate function package implements the individual univariate functions, their convolutions, and reflections. It contains the following classes/interfaces:

 AbstractUnivariate: This abstract class provides the evaluation of the given basis/objective function and its derivatives for a specified variate. Default implementations of the derivatives are for black-box, non-analytical functions.

- 2. <u>UnivariateConvolution</u>: This class provides the evaluation of the point value and the derivatives of the convolution of 2 univariate functions for the specified variate.
- 3. <u>UnivariateReflection</u>: For a given variate x, this class provides the evaluation and derivatives of the reflection at 1-x.
- 4. <u>Polynomial</u>: This class provides the evaluation of the n<sup>th</sup> order polynomial and its derivatives for a specified variate. The degree n specifies the order of the polynomial.
- 5. <u>BernsteinPolynomial</u>: This class provides the evaluation of Bernstein polynomial and its derivatives for a specified variate. The degree exponent specifies the order of the Bernstein polynomial.
- 6. <u>NaturalLogSeriesElement</u>: This class provides the evaluation of a single term in the expansion series for the natural log. The exponent parameter specifies which term in the series is being considered.
- 7. <u>ExponentialTension</u>: This class provides the evaluation of exponential tension basis function and its derivatives for a specified variate. It can be customized by the choice of exponent, the base, and the tension parameter.
- 8. <u>HyperbolicTension</u>: This class provides the evaluation of hyperbolic tension basis function and its derivatives for a specified variate. It can be customized by the choice of the hyperbolic function and the tension parameter.
- 9. <u>LinearRationalShapeControl</u>: This class implements the deterministic rational shape control functionality on top of the estimate of the basis splines inside [0,...]) -

Globally  $[x_0,...,x_1)$ :  $y = \frac{1}{1+\lambda x}$  where is the normalized ordinate mapped as

$$x = \frac{x - x_{i-1}}{x_i - x_{i-1}}.$$

- 10. <u>QuadraticRationalShapeControl</u>: This class implements the deterministic rational shape control functionality on top of the estimate of the basis splines inside [0,...1)
  - Globally  $[x_0,...,x_1)$ :  $y = \frac{1}{1 + \lambda x(1-x)}$  where is the normalized ordinate mapped as

$$x = \frac{x - x_{i-1}}{x_i - x_{i-1}}.$$

11. <u>LinearRationalTensionExponential</u>: This class provides the evaluation of the Convolution of the Linear Rational and the Tension Exponential Function and its derivatives for a specified variate.

#### **Univariate Calculus Package (org.drip.quant.calculus)**

The univariate calculus package implements univariate difference based arbitrary order derivative, implements differential control settings, implements several integrand routines, and multivariate Wengert Jacobian.

- 1. <u>DerivativeControl</u>: DerivativeControl provides bumps needed for numerically approximating derivatives. Bumps can be absolute or relative, and they default to a floor.
- 2. <u>Differential</u>: Differential holds the incremental differentials for the variate and the objective functions.
- 3. <u>WengertJacobian</u>: WengertJacobian contains the Jacobian of the given set of Wengert variables to the set of parameters. It exposes the following functionality:
  - Set/Retrieve the Wengert variables
  - Accumulate the Partials
  - Scale the partial entries
  - Merge the Jacobian with another
  - o Retrieve the WengertJacobian elements
  - o Display the contents of the WengertJacobian
- 4. <u>Integrator</u>: Integrator implements the following routines for integrating the objective functions:
  - Linear Quadrature
  - o Mid-Point Scheme
  - Trapezoidal Scheme
  - o Simpson/Simpson38 Schemes
  - o Boole Scheme

#### Spline Parameters Package (org.drip.spline.params)

The spline parameters package implements the segment and stretch level construction, design, penalty, and shape control parameters.

- 1. <u>ResponseScalingShapeControl</u>: This class implements the segment level basis functions proportional adjustment to achieve the desired shape behavior of the response. In addition to the actual shape controller function, it interprets whether the control is applied on a local or global predicate ordinate basis.
- 2. SegmentBasisFlexureConstraint: This class holds the set of fields needed to characterize a single local linear Constraint, expressed linearly as a combination of the local Predictor Ordinates and their corresponding Response Basis Function Realizations. Constraints are expressed as C<sub>j</sub> = ∑<sub>i</sub> W<sub>i</sub>β<sub>i</sub>(x<sub>j</sub>) where x<sub>j</sub> is the predictor ordinate at node j, β<sub>i</sub> is the Coefficient for the Response Basis Function i, W<sub>i</sub> is the weight applied for the Response Basis Function i, and C<sub>j</sub> is the value of constraint j. SegmentBasisFlexureConstraint may be viewed as the localized basis function transpose of SegmentResponseValueConstraint.
- 3. <u>SegmentResponseValueConstraint</u>: This class holds the following set of fields that characterize a single global linear constraint between the predictor and the response variables within a single segment, expressed linearly across the constituent nodes. SegmentBasisFlexureConstraint may be viewed as the localized basis function transpose of SegmentResponseValueConstraint. SegmentResponseValueConstraint exports the following functionality:
  - Retrieve the Array of Predictor Ordinates
  - o Retrieve the Array of Response Weights at each Predictor Ordinate.
  - o Retrieve the Constraint Value
  - Convert the Segment Constraint onto Local Predictor Ordinates, the corresponding Response Basis Function, and the Shape Controller Realizations
  - Get the Position of the Predictor Knot relative to the Constraints

- Generate a SegmentResponseValueConstraint instance from the given predictor/response pair
- SegmentResponseConstraintSet: This class holds the set of
   SegmentResponseValueConstraint (Base + One/more Sensitivities) for the given
   Segment. It exposes functions to add/retrieve the base response value constraints as
   well as additional response value constraint sensitivities.
- 6. <u>SegmentBestFitResponse</u>: This class implements basis per-segment Fitness Penalty Parameter Set. Currently it contains the Best Fit Penalty Weight Grid Matrix and the corresponding Segment Local Predictor Ordinate/Response Match Pair.
- 7. <u>StretchBestFitResponse</u>: This class implements basis per-Stretch Fitness Penalty Parameter Set. Currently it contains the Best Fit Penalty Weight Grid Matrix and the corresponding Local Predictor Ordinate/Response Match Pair.

StretchBestFitResponse exports the following methods:

- o Retrieve the Array of the Fitness Weights
- Retrieve the Indexed Fitness Weight Element
- Retrieve the Array of Predictor Ordinates
- o Retrieve the Indexed Predictor Ordinate Element
- Retrieve the Array of Responses
- Retrieve the Indexed Response Element
- o Retrieve the Number of Fitness Points
- Generate the Segment Local Best Fit Weighted Response contained within the specified Segment
- o Construct the StretchBestFitResponse Instance from the given Inputs
- Construct the StretchBestFitResponse Instance from the given Predictor
   Ordinate/Response Pairs, using Uniform Weightings
- 8. <u>SegmentFlexurePenaltyControl</u>: This class implements basis per-segment Flexure Penalty Parameter Set. Currently it contains the Flexure Penalty Derivative Order and the Roughness Coefficient Amplitude. Flexure Penalty Control may be used to implement Segment Curvature Control and/or Segment Length Control.
- 9. <u>SegmentDesignInelasticControl</u>: This class implements basis per-segment inelastic parameter set. It exports the following functionality:

- o Retrieve the Continuity Order
- o Retrieve the Length Penalty and the Curvature Penalty Parameters
- Create the  $C^2$  Design Inelastic Parameters
- $\circ$  Create the Design Inelastic Parameters for the desired  $C^k$  Criterion and the Roughness Penalty Order
- 10. <u>SegmentCustomBuilderControl</u>: This class holds the parameters the guide the creation/behavior of the segment. It holds the segment elastic/inelastic parameters and the named basis function set.
- 11. <u>SegmentPredictorResponseDerivative</u>: This class contains the segment local parameters used for the segment calibration. It holds the edge Input Response value and its derivatives. It exposes the following functions:
  - o Retrieve the Response Value as well as the DResponseDPredictorOrdinate Array
  - Aggregate the 2 Predictor Ordinate Response Derivatives by applying the Cardinal Tension Weight
- 12. <u>SegmentStateCalibration</u>: This class implements basis per-segment Calibration Parameter Set. It exposes the following functionality:
  - Retrieve the Array of the Calibration Predictor Ordinates
  - o Retrieve the Array of the Calibration Response Values
  - o Retrieve the Array of the Left/Right Edge Derivatives
  - Retrieve the Segment Best Fit Response
  - o Retrieve the Array of Segment Basis Flexure Constraints

### Spline Basis Function Set Package (org.drip.spline.basis)

The spline basis function set package implements the basis set, parameters for the different basis functions, parameters for basis set construction, and parameters for B Spline sequence construction.

- 1. <u>FunctionSet</u>: This class implements the general-purpose basis spline function set.
- 2. <u>FunctionSetBuilderParams</u>: This is an empty stub class whose derived implementations hold the per-segment basis set parameters.

- 3. <u>ExponentialMixtureSetParams</u>: ExponentialMixtureSetParams implements persegment parameters for the exponential mixture basis set the array of the exponential tension parameters, one per each entity in the mixture.
- 4. <u>ExponentialTensionSetParams</u>: ExponentialTensionSetParams implements persegment parameters for the exponential tension basis set currently it only contains the tension parameter.
- 5. <u>ExponentialRationalSetParams</u>: ExponentialRationalSetParams implements persegment parameters for the exponential rational basis set the exponential tension and the rational tension parameters.
- 6. <u>PolynomialFunctionSetParams</u>: PolynomialFunctionSetParams implements persegment basis set parameters for the polynomial basis spline currently it holds the number of basis functions.
- 7. <u>KaklisPandelisSetParams</u>: KaklisPandelisSetParams implements per-segment parameters for the Kalkis-Pandelis basis set currently it only holds the polynomial tension degree.
- 8. <u>FunctionSetBuilder</u>: This class implements the basis set and spline builder for the following types of splines:
  - Exponential basis tension splines
  - Hyperbolic basis tension splines
  - Polynomial basis splines
  - Bernstein Polynomial basis splines
  - Kaklis-Pandelis basis tension splines

The elastic coefficients for the segment using  $C^k$  basis splines inside [0,...,1) - globally  $[x_0,...,x_1)$ :  $y = BasisSplineFunction(C^k,x) \times ShapeController(x)$  where is the normalized ordinate mapped as  $x = \frac{x - x_{i-1}}{x_i - x_{i-1}}$ . The inverse quadratic/rational spline is a typical shape controller spline used.

- 9. <u>BSplineSequenceParams</u>: BSplineSequenceParams implements the parameter set for constructing the B Spline Sequence. It provides functionality to:
  - o Retrieve the B Spline Order
  - Retrieve the Number of Basis Functions

- Retrieve the Processed Basis Derivative Order
- Retrieve the Basis Hat Type
- Retrieve the Shape Control Type
- o Retrieve the Tension
- Retrieve the Array of Predictor Ordinates

#### Spline Segment Package (org.drip.spline.segment)

The spline segment package implements the segment's inelastic state, the segment basis evaluator, the segment flexure penalizer, computes the segment monotonicity behavior, and implements the segment's complete constitutive state.

- 1. <u>InelasticConstitutiveState</u>: This class contains the spline segment in-elastic fields in this case the start/end ranges. It exports the following functions:
  - Retrieve the Segment Left/Right Predictor Ordinate
  - Find out if the Predictor Ordinate is inside the segment inclusive of left/right
  - Get the Width of the Predictor Ordinate in this Segment
  - Transform the Predictor Ordinate to the Local Segment Predictor Ordinate
  - Transform the Local Predictor Ordinate to the Segment Ordinate
- 2. <u>BasisEvaluator</u>: This interface implements the Segment's Basis Evaluator Functions. It exports the following functions:
  - Retrieve the number of Segment's Basis Functions
  - Set the Inelastics that provides the enveloping Context the Basis Evaluation
  - Clone/Replicate the current Basis Evaluator Instance
  - Compute the Response Value of the indexed Basis Function at the specified Predictor Ordinate
  - Compute the Basis Function Value at the specified Predictor Ordinate
  - Compute the Response Value at the specified Predictor Ordinate
  - Compute the Ordered Derivative of the Response Value off of the indexed Basis Function at the specified Predictor Ordinate

- Compute the Ordered Derivative of the Response Value off of the Basis Function
   Set at the specified Predictor Ordinate
- Compute the Response Value Derivative at the specified Predictor Ordinate
- 3. <u>SegmentBasisEvaluator</u>: This class implements the BasisEvaluator interface for the given Set of the Segment Basis Evaluator Functions.
- 4. <u>Monotonicity</u>: This class contains the monotonicity details related to the given segment. It computes whether the segment is monotonic, and if not, whether it contains a maximum, a minimum, or an inflection.
- 5. <u>BestFitFlexurePenalizer</u>: This Class implements the Segment's Best Fit, Curvature, and Length Penalizers. It provides the following functionality:
  - Compute the Cross-Curvature Penalty for the given Basis Pair
  - Compute the Cross-Length Penalty for the given Basis Pair
  - Compute the Best Fit Cross-Product Penalty for the given Basis Pair
  - Compute the Basis Pair Penalty Coefficient for the Best Fit and the Curvature Penalties
  - Compute the Penalty Constraint for the Basis Pair
- 6. <u>ConstitutiveState</u>: ConstitutiveState implements the single segment basis calibration and inference functionality. It exports the following functionality:
  - Build the ConstitutiveState instance from the Basis Function/Shape Controller Set
  - Build the ConstitutiveState instance from the Basis Evaluator Set
  - Retrieve the Number of Parameters, Basis Evaluator, Array of the Response Basis
     Coefficients, and Segment Design Inelastic Control
  - Calibrate the Segment State from the Calibration Parameter Set
  - Sensitivity Calibrator: Calibrate the Segment Quote Jacobian from the Calibration Parameter Set
  - Calibrate the coefficients from the prior Predictor/Response Segment, the Constraint, and fitness Weights
  - Calibrate the coefficients from the prior Segment and the Response Value at the Right Predictor Ordinate
  - Calibrate the Coefficients from the Edge Response Values and the Left Edge Response Slope

- Calibrate the coefficients from the Left Edge Response Value Constraint, the Left
   Edge Response Value Slope, and the Right Edge Response Value Constraint
- Retrieve the Segment Curvature, Length, and the Best Fit DPE
- Calculate the Response Value and its Derivative at the given Predictor Ordinate
- Calculate the Ordered Derivative of the Coefficient to the Quote
- Calculate the Jacobian of the Segment's Response Basis Function Coefficients to the Edge Inputs
- Calculate the Jacobian of the Response to the Edge Inputs at the given Predictor Ordinate
- Calculate the Jacobian of the Response to the Basis Coefficients at the given Predictor Ordinate
- Calibrate the segment and calculate the Jacobian of the Segment's Response Basis
   Function Coefficients to the Edge Parameters
- Calibrate the Coefficients from the Edge Response Values and the Left Edge Response Value Slope and calculate the Jacobian of the Segment's Response Basis Function Coefficients to the Edge Parameters
- Calibrate the coefficients from the prior Segment and the Response Value at the Right Predictor Ordinate and calculate the Jacobian of the Segment's Response Basis Function Coefficients to the Edge Parameters
- Indicate whether the given segment is monotone. If monotone, may optionally indicate the nature of the extrema contained inside maxima/minima/infection)
- Clip the part of the Segment to the Right of the specified Predictor Ordinate.
   Retain all other constraints the same
- Clip the part of the Segment to the Left of the specified Predictor Ordinate. Retain all other constraints the same
- Display the string representation for diagnostic purposes

### **Spline Stretch Package (org.drip.spline.stretch)**

The spline stretch package provides single segment and multi segment interfaces, builders, and implementations, along with custom boundary settings.

- 1. <u>BoundarySettings</u>: This class implements the Boundary Settings that determine the full extent of description of the stretch's State. It exports functions that:
  - Specify the type of the boundary condition (NATURAL/FLOATING/IS-A-KNOT)
  - Boundary Condition specific additional parameters (e.g., Derivative Orders and Matches)
  - Static methods that help construct standard boundary settings
- 2. <u>SingleSegmentSequence</u>: SingleSegmentSequence is the interface that exposes functionality that spans multiple segments. Its derived instances hold the ordered segment sequence, the segment control parameters, and, if available, the spanning Jacobian. SingleSegmentSequence exports the following group of functionality:
  - Construct adjoining segment sequences in accordance with the segment control parameters
  - Calibrate according to a varied set of (i.e., NATURAL/FINANCIAL) boundary conditions
  - Estimate both the value, the ordered derivatives, and the Jacobian (quote/coefficient) at the given ordinate
  - Compute the monotonicity details segment/Stretch level monotonicity, comonotonicity, local monotonicity.
  - Predictor Ordinate Details identify the left/right predictor ordinate edges, and whether the given predictor ordinate is a knot
- 3. <u>SingleSegmentLagrangePolynomial</u>: SingleSegmentLagrangePolynomial implements the SingleSegmentSequence Stretch interface using the Lagrange Polynomial Estimator. As such it provides a perfect fit that travels through all the predictor/response pairs causing Runge's instability.
- 4. <u>MultiSegmentSequence</u>: MultiSegmentSequence is the interface that exposes functionality that spans multiple segments. Its derived instances hold the ordered segment sequence, the segment control parameters, and, if available, the spanning Jacobian. MultiSegmentSequence exports the following group of functionality:

- Retrieve the Segments and their Builder Parameters
- Compute the monotonicity details segment/Stretch level monotonicity, comonotonicity, local monotonicity
- Check if the Predictor Ordinate is in the Stretch Range, and return the segment index in that case
- Set up (i.e., calibrate) the individual Segments in the Stretch by specifying one/or more of the node parameters and Target Constraints
- Set up (i.e., calibrate) the individual Segment in the Stretch to the Target Segment Edge Values and Constraints. This is also called the Hermite setup where the segment boundaries are entirely locally set
- Generate a new Stretch by clipping all the Segments to the Left/Right of the specified Predictor Ordinate. Smoothness Constraints will be maintained.
- Retrieve the Span Curvature/Length, and the Best Fit DPE's
- Retrieve the Merge Stretch Manager
- Display the Segments
- 5. <u>SegmentSequenceBuilder</u>: SegmentSequenceBuilder is the interface that contains the stubs required for the construction of the segment stretch. It exposes the following functions:
  - Set the Stretch whose Segments are to be calibrated
  - Retrieve the Calibration Boundary Condition
  - Calibrate the Starting Segment using the Left Slope
  - Calibrate the Segment Sequence in the Stretch
- 6. <u>CkSegmentSequenceBuilder</u>: CkSegmentSequenceBuilder implements the SegmentSequenceBuilder interface to customize segment sequence construction. Customization is applied at several levels:
  - Segment Calibration Boundary Setting/Segment Best Fit Response Settings
  - Segment Response Value Constraints for the starting and the subsequent Segments
- 7. <u>CalibratableMultiSegmentSequence</u>: CalibratableMultiSegmentSequence implements the MultiSegmentSequence span that spans multiple segments. It holds the ordered segment sequence, segment sequence builder, the segment control parameters, and, if

- available, the spanning Jacobian. It provides a variety of customization for the segment construction and state representation control.
- 8. <u>MultiSegmentSequenceBuilder</u>: MultiSegmentSequenceBuilder exports Stretch creation/calibration methods to generate customized basis splines, with customized segment behavior using the segment control. It exports the following methods of Stretch Creation:
  - Create an uncalibrated Stretch instance over the specified Predictor Ordinate
     Array using the specified Basis Spline Parameters for the Segment
  - Create a calibrated Stretch Instance over the specified array of Predictor Ordinates and Response Values using the specified Basis Splines
  - Create a calibrated Stretch Instance over the specified Predictor Ordinates,
     Response Values, and their constraints, using the specified Segment Builder
     Parameters
  - Create a Calibrated Stretch Instance from the Array of Predictor Ordinates and a flat Response Value
  - Create a Regression Spline Instance over the specified array of Predictor Ordinate
     Knot Points and the Set of the Points to be Best Fit
- 9. <u>MultiSegmentSequenceModifier</u>: MultiSegmentSequenceModifier exports Stretch modification/alteration methods to generate customized basis splines, with customized segment behavior using the segment control. It exposes the following stretch modification methods:
  - Insert the specified Predictor Ordinate Knot into the specified Stretch, using the specified Response Value
  - Append a Segment to the Right of the Specified Stretch using the Supplied Constraint
  - Insert the Predictor Ordinate Knot into the specified Stretch
  - Insert a Cardinal Knot into the specified Stretch at the specified Predictor Ordinate Location
  - Insert a Catmull-Rom Knot into the specified Stretch at the specified Predictor Ordinate Location

#### Spline Grid/Span Package (org.drip.spline.grid)

The spline grid/span package provides the multi-stretch spanning functionality. It specifies the span interface, and provides implementations of the overlapping and the non-overlapping span instances. It also implements the transition splines with custom transition zones.

- 1. <u>Span</u>: Span is the interface that exposes the functionality behind the collection of Stretches that may be overlapping or non-overlapping. It exposes the following stubs:
  - Retrieve the Left/Right Span Edge
  - Indicate if the specified Label is part of the Merge State at the specified Predictor Ordinate
  - Compute the Response from the containing Stretches
  - Add a Stretch to the Span
  - Retrieve the first Stretch that contains the Predictor Ordinate
  - Retrieve the Stretch by Name
  - Calculate the Response Derivative to the Quote at the specified Ordinate
  - Display the Span Edge Coordinates
- 2. OverlappingStretchSpan: OverlappingStretchSpan implements the Span interface, and the collection functionality of overlapping Stretches. In addition to providing a custom implementation of all the Span interface stubs, it also converts the Overlapping Stretch Span to a non-overlapping Stretch Span. Overlapping Stretches are clipped from the Left.

### **Spline PCHIP Package (org.drip.spline.pchip)**

The spline PCHIP package implements most variants of the local piece-wise cubic Hermite interpolating polynomial smoothing functionality. It provides a number of tweaks for smoothing customization, as well as providing enhanced implementations of Akima, Preuss, and Hagan-West smoothing interpolators.

- 1. <u>AkimaLocalC1Generator</u>: AkimaLocalC1Generator generates the local control  $C^1$  Slope using the Akima (1970) Cubic Algorithm.
- 2. <u>MinimalQuadraticHaganWest</u>: This class implements the regime using the Hagan and West (2006) Minimal Quadratic Estimator.
- 3. <u>MonotoneConvexHaganWest</u>: This class implements the regime using the Hagan and West (2006) Estimator. It provides the following functionality:
  - Static Method to create an instance of MonotoneConvexHaganWest
  - Ensure that the estimated regime is monotone an convex
  - If need be, enforce positivity and/or apply amelioration
  - Apply segment-by-segment range bounds as needed
  - Retrieve predictor ordinates/response values
- 4. <u>LocalMonotoneCkGenerator</u>: LocalMonotoneCkGenerator generates customized Local Stretch by trading off  $C^k$  for local control. This class implements the following variants: Akima, Bessel, Harmonic, Hyman83, Hyman89, Kruger, Monotone Convex, as well as the Van Leer and the Huynh/Le Floch limiters. It also provides the following custom control on the resulting  $C^1$ :
  - Eliminate the Spurious Extrema in the Input  $C^1$  Entry
  - Apply the Monotone Filter in the Input  $C^1$  Entry
  - Generate a Vanilla  $C^1$  Array from the specified Array of Predictor Ordinates and the Response Values
  - Verify if the given Quintic Polynomial is Monotone using the Hyman89
     Algorithm, and generate it if necessary
- 5. <u>LocalControlStretchBuilder</u>: LocalControlStretchBuilder exports Stretch creation/calibration methods to generate customized basis splines, with customized segment behavior using the segment control. It provides the following local-control functionality:
  - Create a Stretch off of Hermite Splines from the specified the Predictor Ordinates, the Response

- Values, the Custom Slopes, and the Segment Builder Parameters
- Create Hermite/Bessel C1 Cubic Spline Stretch
- Create Hyman (1983) Monotone Preserving Stretch
- Create Hyman (1989) enhancement to the Hyman (1983) Monotone Preserving Stretch
- Create the Harmonic Monotone Preserving Stretch
- Create the Van Leer Limiter Stretch
- Create the Huynh Le Floch Limiter Stretch
- Generate the local control C1 Slope using the Akima Cubic Algorithm
- Generate the local control C1 Slope using the Hagan-West Monotone Convex Algorithm

#### Spline B Spline Package (org.drip.spline.bspline)

The spline B Spline package implements the raw and the processed basis B Spline hat functions. It provides the standard implementations for the monic and the multic B Spline Segments. It also exports functionality to generate higher order B Spline Sequences.

- 1. <u>TensionBasisHat</u>: TensionBasisHat implements the common basis hat function that forms the basis for all B Splines. It contains the left/right ordinates, the tension, and the normalizer.
- TensionProcessedBasisHat: TensionProcessedBasisHat implements the processed hat basis function of the form laid out in the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000).
- 3. <u>BasisHatShapeControl</u>: BasisHatShapeControl implements the shape control function for the hat basis set as laid out in the framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000). Currently BasisHatShapeControl implements the following shape control customizers:
  - a. Cubic Polynomial with Rational Linear Shape Controller
  - b. Cubic Polynomial with Rational Quadratic Shape Controller
  - c. Cubic Polynomial with Rational Exponential Shape Controller

- 4. <u>LeftHatShapeControl</u>: LeftHatShapeControl implements the BasisHatShapeControl interface for the left hat basis set as laid out in the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000).
- RightHatShapeControl: RightHatShapeControl implements the BasisHatShapeControl interface for the right hat basis set as laid out in the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000).
- CubicRationalLeftRaw: CubicRationalLeftRaw implements the TensionBasisHat
  interface in accordance with the raw left cubic rational hat basis function laid out in
  the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and
  Kvasov (2000).
- CubicRationalRightRaw: CubicRationalRightRaw implements the TensionBasisHat
  interface in accordance with the raw right cubic rational hat basis function laid out in
  the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and
  Kvasov (2000).
- 8. ExponentialTensionLeftHat: ExponentialTensionLeftHat implements the TensionBasisHat interface in accordance with the left exponential hat basis function laid out in the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000).
- 9. ExponentialTensionRightHat: ExponentialTensionRightHat implements the TensionBasisHat interface in accordance with the right exponential hat basis function laid out in the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000).
- 10. <u>ExponentialTensionLeftRaw</u>: ExponentialTensionLeftRaw implements the TensionBasisHat interface in accordance with the raw left exponential hat basis function laid out in the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000).
- 11. ExponentialTensionRightRaw: ExponentialTensionRightRaw implements the TensionBasisHat interface in accordance with the raw right exponential hat basis function laid out in the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000).

- 12. <u>BasisHatPairGenerator</u>: BasisHatPairGenerator implements the generation functionality behind the hat basis function pair. It provides the following functionality:
  - a. Generate the array of the Hyperbolic Phy and Psy Hat Function Pair
  - b. Generate the array of the Hyperbolic Phy and Psy Hat Function Pair From their Raw Counterparts
  - c. Generate the array of the Cubic Rational Phy and Psy Hat Function Pair From their Raw Counterparts
  - d. Generate the array of the Custom Phy and Psy Hat Function Pair From their Raw Counterparts
- 13. <u>SegmentBasisFunction</u>: SegmentBasisFunction is the abstract class over which the local ordered envelope functions for the B Splines are implemented. It exposes the following stubs:
  - a. Retrieve the Order of the B Spline
  - b. Retrieve the Leading Predictor Ordinate
  - c. Retrieve the Following Predictor Ordinate
  - d. Retrieve the Trailing Predictor Ordinate
  - e. Compute the complete Envelope Integrand this will serve as the Envelope Normalizer
  - f. Evaluate the Cumulative Normalized Integrand up to the given ordinate
- 14. <u>SegmentMonicBasisFunction</u>: SegmentMonicBasisFunction implements the local monic B Spline that envelopes the predictor ordinates, and the corresponding set of ordinates/basis functions. SegmentMonicBasisFunction uses the left/right TensionBasisHat instances to achieve its implementation goals.
- 15. <u>SegmentMulticBasisFunction</u>: SegmentMulticBasisFunction implements the local multic B Spline that envelopes the predictor ordinates, and the corresponding set of ordinates/basis functions. SegmentMulticBasisFunction uses the left/right SegmentBasisFunction instances to achieve its implementation goals.
- 16. <u>SegmentBasisFunctionSet</u>: SegmentBasisFunctionSet class implements per-segment function set for B Splines and tension splines. Derived implementations expose explicit targeted basis functions.

- 17. <u>SegmentBasisFunctionGenerator</u>: SegmentBasisFunctionGenerator generates B Spline Functions of different order. It provides the following functionality:
  - a. Create a Tension Monic B Spline Basis Function
  - b. Construct a Sequence of Monic Basis Functions
  - c. Create a sequence of B Splines of the specified order from the given inputs

#### **Tension Spline Package (org.drip.spline.tension)**

The tension spline package implements closed form family of cubic tension splines laid out in the basic framework outlined in Koch and Lyche (1989), Koch and Lyche (1993), and Kvasov (2000).

- 1. <u>KLKHyperbolicTensionPhy</u>: KLKHyperbolicTensionPhy implements the custom evaluator, differentiator, and integrator for the KLK Tension Phy Functions outlined in the publications above.
- 2. <u>KLKHyperbolicTensionPsy</u>: KLKHyperbolicTensionPsy implements the custom evaluator, differentiator, and integrator for the KLK Tension Psy Functions outlined in the publications above.
- 3. <u>KochLycheKvasovBasis</u>: This class exposes functions that implement the monic, quadratic, and the cubic basis B Splines as outlined in the publications above.
- 4. <u>KochLycheKvasovFamily</u>: This class implements the basic framework and the family of  $C^2$  Tension Splines outlined above. Functions exposed here implement the Basis Function Set from:
  - a. Hyperbolic Hat Primitive Set
  - b. Cubic Polynomial Numerator and Linear Rational Denominator
  - c. Cubic Polynomial Numerator and Quadratic Rational Denominator
  - d. Cubic Polynomial Numerator and Exponential Denominator

#### **Spline Sample Package (org.drip.sample.spline)**

The spline sample package contains samples that demonstrate the construction and usage of different basis splines and B Spline Sequences.

- 1. <u>BasisSplineSet</u>: BasisSplineSet implements Samples for the Construction and the usage of various basis spline functions. It demonstrates the following:
  - a. Construction of segment control parameters polynomial (regular/Bernstein) segment control, exponential/hyperbolic tension segment control, Kaklis-Pandelis tension segment control, and  $C^1$  Hermite
  - b. Control the segment using the rational shape controller, and the appropriate  $C^k$
  - c. Estimate the node value and the node value Jacobian with the segment, as well as at the boundaries
  - d. Calculate the segment monotonicity
- PolynomialBasisSpline: PolynomialBasisSpline implements Samples for the Construction and the usage of polynomial (both regular and Hermite) basis spline functions. It demonstrates the following:
  - a. Control the polynomial segment using the rational shape controller, the appropriate  $C^k$ , and the basis function
  - b. Demonstrate the variational shape optimization behavior
  - c. Estimate the node value and the node value Jacobian with the segment, as well as at the boundaries
  - d. Calculate the segment monotonicity and the curvature penalty
- 3. <u>BasisTensionSplineSet</u>: BasisTensionSplineSet implements Samples for the Construction and the usage of various basis spline functions. It demonstrates the following:
  - Construction of Kocke-Lyche-Kvasov tension spline segment control parameters - using hyperbolic, exponential, rational linear, and rational quadratic primitives
  - b. Control the segment using the rational shape controller, and the appropriate  $C^k$
  - c. Estimate the node value and the node value Jacobian with the segment, as well as at the boundaries

- d. Calculate the segment monotonicity
- 4. <u>BasisBSplineSet</u>: BasisBSplineSet implements Samples for the Construction and the usage of various basis B Spline functions.
- 5. <u>BasisMonicHatComparison</u>: BasisMonicHatComparison implements the comparison of the basis hat functions used in the construction of the monic basis B Splines. It demonstrates the following:
  - a. Construction of the Linear Cubic Rational Raw Hat Functions
  - b. Construction of the Ouadratic Cubic Rational Raw Hat Functions
  - c. Construction of the Corresponding Processed Tension Basis Hat Functions
  - d. Construction of the Wrapping Monic Functions
  - e. Estimation and Comparison of the Ordered Derivatives
- 6. <u>BasisMonicBSpline</u>: BasisMonicBSpline implements Samples for the Construction and the usage of various monic basis B Splines. It demonstrates the following:
  - a. Construction of segment B Spline Hat Basis Functions
  - b. Estimation of the derivatives and the basis envelope cumulative integrands
  - c. Estimation of the normalizer and the basis envelope cumulative normalized integrand
- 7. <u>BasisMulticBSpline</u>: BasisMulticBSpline implements Samples for the Construction and the usage of various multic basis B Splines. It demonstrates the following:
  - a. Construction of segment higher order B Spline Hat Basis Functions
  - b. Estimation of the derivatives and the basis envelope cumulative integrands
  - c. Estimation of the normalizer and the basis envelope cumulative normalized integrand
- 8. <u>BSplineSequence</u>: BSplineSequence implements Samples for the Construction and the usage of various monic basis B Spline Sequences. It demonstrates the following:
  - a. Construction and Usage of segment Monic B Spline Sequence
  - b. Construction and Usage of segment Multic B Spline Sequence

#### Stretch Sample Package (org.drip.sample.stretch)

The stretch sample package contains samples that demonstrate the construction, modification, and usage of stretches based off of different basis splines. They illustrate the computation of the curvature and the length penalties, and construction of best fit regression spline samples. Finally they bring it all together in showing how to build latent state from measurements.

- 1. <u>StretchEstimation</u>: StretchEstimation demonstrates the Stretch builder and usage API. It shows the following:
  - a. Construction of segment control parameters polynomial (regular/Bernstein)
     segment control, exponential/hyperbolic tension segment control, Kaklis Pandelis tension segment control
  - Perform the following sequence of tests for a given segment control for a predictor/response range
    - i. Assign the array of Segment Builder Parameters one per segment
    - ii. Construct the Stretch Instance
    - iii. Estimate, compute the segment-by-segment monotonicity and the Stretch Jacobian
    - iv. Construct a new Stretch instance by inserting a pair of predictor/response knots
    - v. Estimate, compute the segment-by-segment monotonicity and the Stretch Jacobian
  - c. Demonstrate the construction, the calibration, and the usage of Local Control Segment Spline
  - d. Demonstrate the construction, the calibration, and the usage of Lagrange Polynomial Stretch
  - e. Demonstrate the construction, the calibration, and the usage of C1 Stretch with the desired customization.
- 2. <u>TensionStretchEstimation</u>: TensionStretchEstimation demonstrates the Stretch builder and usage API. It shows the following:
  - a. Construction of segment control parameters polynomial (regular/Bernstein)
     segment control, exponential/hyperbolic tension segment control, Kaklis Pandelis tension segment control

- b. Tension Basis Spline Test using the specified predictor/response set and the array of segment custom builder control parameters
- c. Complete the full tension stretch estimation sample test
- 3. <u>StretchAdjuster</u>: StretchAdjuster demonstrates the Stretch Manipulation and Adjustment API. It shows the following:
  - a. Construct a simple Base Stretch
  - b. Clip a left Portion of the Stretch to construct a left-clipped Stretch
  - c. Clip a right Portion of the Stretch to construct a tight-clipped Stretch
  - d. Compare the values across all the stretches to establish a) the continuity in the base smoothness is, preserved, and b) Continuity across the predictor ordinate for the implied response value is also preserved
- 4. <u>RegressionSplineEstimator</u>: RegressionSplineEstimator shows the sample construction and usage of Regression Splines. It demonstrates the construction of the segment's predictor ordinate/response value combination, and eventual calibration.
- 5. <u>PenalizedCurvatureFit</u>: PenalizedCurvatureFit demonstrates the setting up and the usage of the curvature and closeness of fit penalizing spline. It illustrates in detail the following steps:
  - a. Set up the X Predictor Ordinate and the Y Response Value Set
  - b. Construct a set of Predictor Ordinates, their Responses, and corresponding
     Weights to serve as weighted closeness of fit
  - c. Construct a rational shape controller with the desired shape controller tension parameters and Global Scaling
  - d. Construct the segment inelastic parameter that is C2, with 2nd order roughness penalty derivative, and without constraint
  - e. Construct the base, the base + 1 degree segment builder control
  - f. Construct the base, the elevated, and the best fit basis spline stretches
  - g. Compute the segment-by-segment monotonicity for all the three stretches
  - h. Compute the Stretch Jacobian for all the three stretches
  - i. Compute the Base Stretch Curvature Penalty Estimate
  - j. Compute the Elevated Stretch Curvature Penalty Estimate
  - k. Compute the Best Fit Stretch Curvature Penalty Estimate

- 6. <u>PenalizedCurvatureLengthFit</u>: PenalizedCurvatureLengthFit demonstrates the setting up and the usage of the curvature, the length, and the closeness of fit penalizing spline. This sample shows the following:
  - a. Set up the X Predictor Ordinate and the Y Response Value Set
  - b. Construct a set of Predictor Ordinates, their Responses, and corresponding
     Weights to serve as weighted closeness of fit
  - c. Construct a rational shape controller with the desired shape controller tension parameters and Global Scaling
  - d. Construct the Segment Inelastic Parameter that is C2, with First Order Segment Length Penalty Derivative, Second Order Segment Curvature Penalty Derivative, their Amplitudes, and without Constraint
  - e. Construct the base, the base + 1 degree segment builder control
  - f. Construct the base, the elevated, and the best fit basis spline stretches
  - g. Compute the segment-by-segment monotonicity for all the three stretches
  - h. Compute the Stretch Jacobian for all the three stretches
  - i. Compute the Base Stretch Curvature, Length, and the Best Fit DPE
  - j. Compute the Elevated Stretch Curvature, Length, and the Best Fit DPE
  - k. Compute the Best Fit Stretch Curvature, Length, and the Best Fit DPE
- 7. <u>CustomCurveBuilder</u>: CustomCurveBuilder contains samples that demo how to build a discount curve from purely the cash flows. It provides for elaborate curve builder control, both at the segment level and at the Stretch level. In particular, it shows the following:
  - a. Construct a discount curve from the discount factors available purely from the cash and the euro-dollar instruments
  - b. Construct a discount curve from the cash flows available from the swap instruments

In addition, the sample demonstrates the following ways of controlling curve construction:

- Control over the type of segment basis spline
- Control over the polynomial basis spline order  $C^k$ , and tension parameters
- Provision of custom shape controllers (in this case rational shape controller)

Calculation of segment monotonicity and convexity

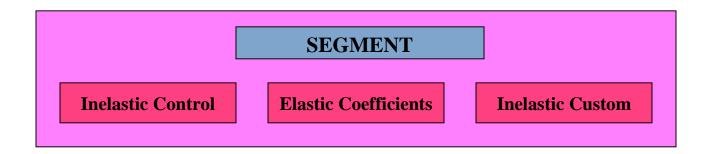
#### Spline/Stretch Regression Test Package (org.drip.regression.spline)

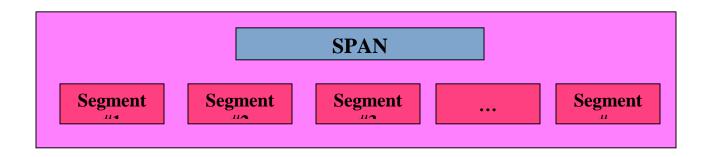
This package contains the random input regression runs on the spline and stretch instances. Runs regress on C1Hermite, local control smoothing, single segment Lagrangians, multi-segment sequences using a variety of spline/stretch basis functions and controls.

- BasisSplineRegressor: BasisSplineRegressor implements the custom basis spline regressor for the given basis spline. As part of the regression sequence, it executes the following:
  - a. Calibrate and compute the left and the right Jacobian
  - b. Reset right node and re-run calibration
  - c. Compute an intermediate value Jacobian
- 2. <u>HermiteBasisSplineRegressor</u>: HermiteBasisSplineRegressor implements the BasisSplineRegressor using the Hermite basis spline regressor.
- LagrangePolynomialStretchRegressor: LagrangePolynomialStretchRegressor
  implements the BasisSplineRegressor using the SingleSegmentLagrangePolynomial
  regressor.
- 4. <u>LocalControlBasisSplineRegressor</u>: LocalControlBasisSplineRegressor implements the local control basis spline regressor for the given basis spline. As part of the regression run, it executes the following:
  - a. Calibrate and compute the left and the right Jacobian
  - b. Insert the Local Control Hermite, Cardinal, and Catmull-Rom knots
  - c. Run Regressor for the C1 Local Control C1 Slope Insertion Bessel/Hermite
     Spline
  - d. Compute an intermediate value Jacobian
- 5. <u>BasisSplineRegressorSet</u>: BasisSplineRegressorSet carries out regression testing for the following series of basis splines:
  - a. Polynomial Basis Spline, n = 2 basis functions, and  $C^1$

- b. Polynomial Basis Spline, n = 3 basis functions, and  $C^1$
- c. Polynomial Basis Spline, n = 4 basis functions, and  $C^1$
- d. Polynomial Basis Spline, n = 4 basis functions, and  $C^2$
- e. Polynomial Basis Spline, n = 5 basis functions, and  $C^1$
- f. Polynomial Basis Spline, n = 5 basis functions, and  $C^2$
- g. Polynomial Basis Spline, n = 5 basis functions, and  $C^3$
- h. Polynomial Basis Spline, n = 6 basis functions, and  $C^1$
- i. Polynomial Basis Spline, n = 6 basis functions, and  $C^2$
- j. Polynomial Basis Spline, n = 6 basis functions, and  $C^3$
- k. Polynomial Basis Spline, n = 6 basis functions, and  $C^4$
- 1. Polynomial Basis Spline, n = 7 basis functions, and  $C^1$
- m. Polynomial Basis Spline, n = 7 basis functions, and  $C^2$
- n. Polynomial Basis Spline, n = 7 basis functions, and  $C^3$
- o. Polynomial Basis Spline, n = 7 basis functions, and  $C^4$
- p. Polynomial Basis Spline, n = 7 basis functions, and  $C^5$
- q. Bernstein Polynomial Basis Spline, n = 4 basis functions, and  $C^2$
- r. Exponential Tension Spline, n = 4 basis functions, Tension = 1., and  $C^2$
- s. Hyperbolic Tension Spline, n = 4 basis functions, Tension = 1., and  $C^2$
- t. Kaklis-Pandelis Tension Spline, n = 4 basis functions, KP = 2, and  $C^2$
- u. C1 Hermite Local Spline, n = 4 basis functions, and  $C^1$
- v. Hermite Local Spline with Local, Catmull-Rom, and Cardinal Knots, n = 4 basis functions, and  $C^1$
- 6. <u>BasisSplineRegressionEngine</u>: BasisSplineRegressionEngine implements the RegressionEngine class for the basis spline regression functionality.

# Figure #1 SEGMENT/SPAN Structure Layout

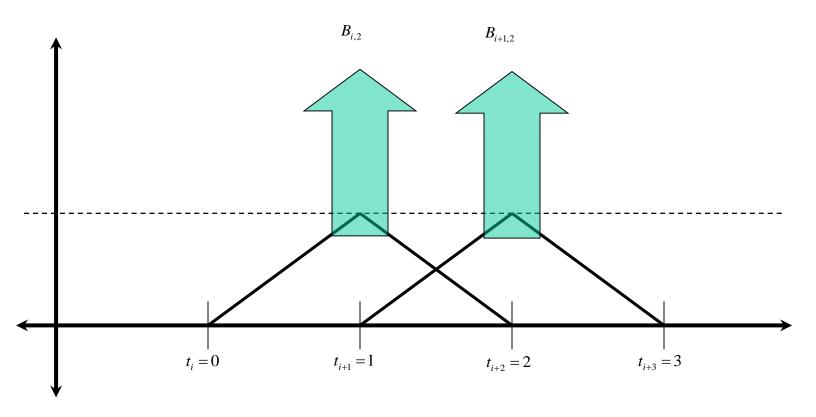




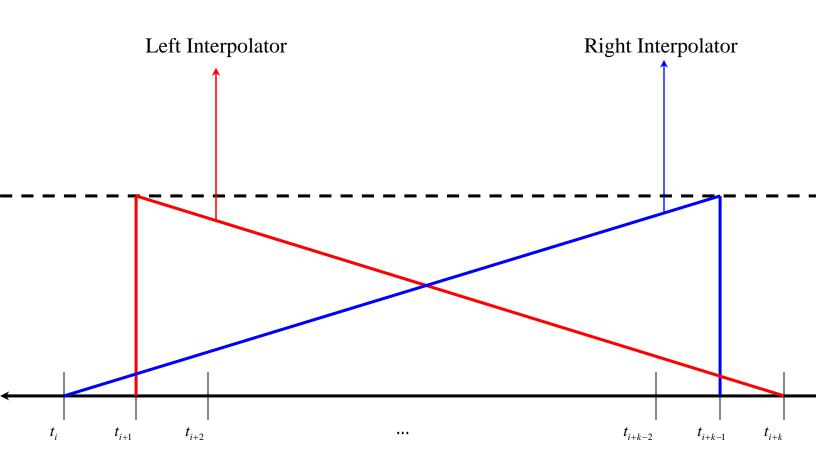
# Figure #2 BASIS SPLINE HIERARCHY

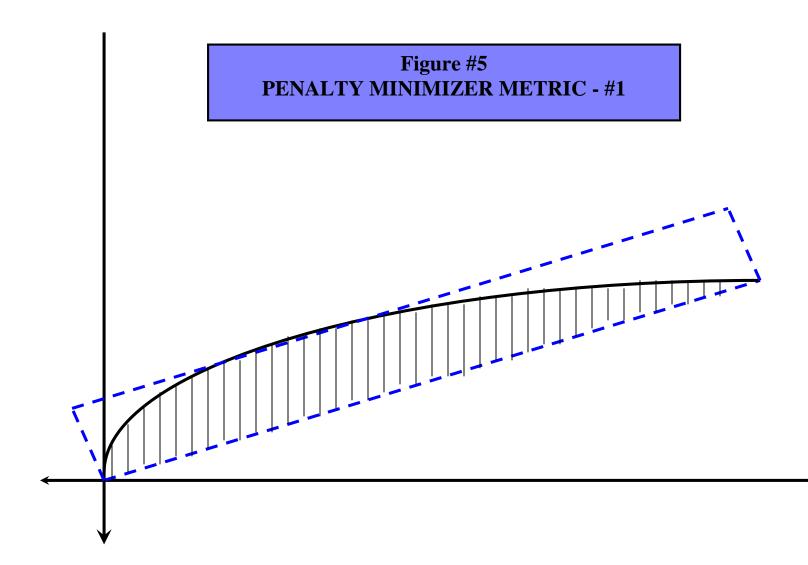
SEGMENT	
Basis Spline Polynomial	<b>Basis Spline Hyperbolic Tension</b>
Basis Spline Linear Polynomial	Basis Spline Exponential Tension
Basis Cubic Polynomial	Basis Spline Cubic Hermite
Basis Quartic Polynomial	<b>Basis Spline Catmull Rom</b>
Basis Cubic Rational  Segment  Segment	

# Figure #3 THIRD ORDER SECOND DEGREE SPLINE

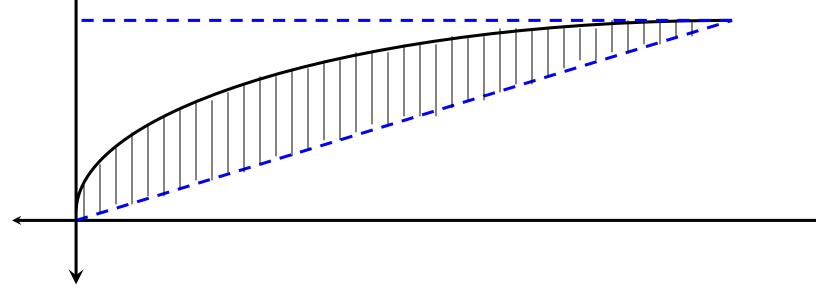


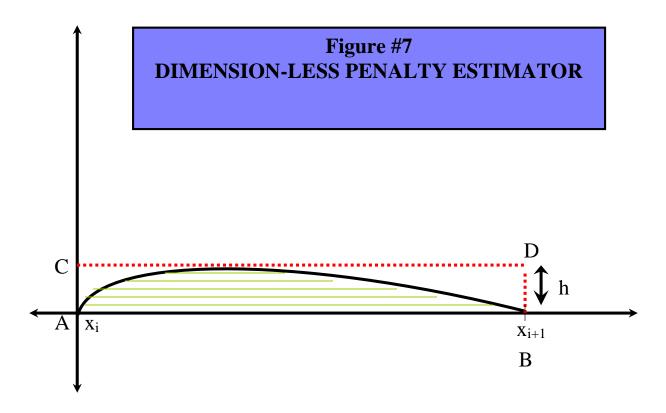
# Figure #4 B SPLINE INTERPLATION SCHEME

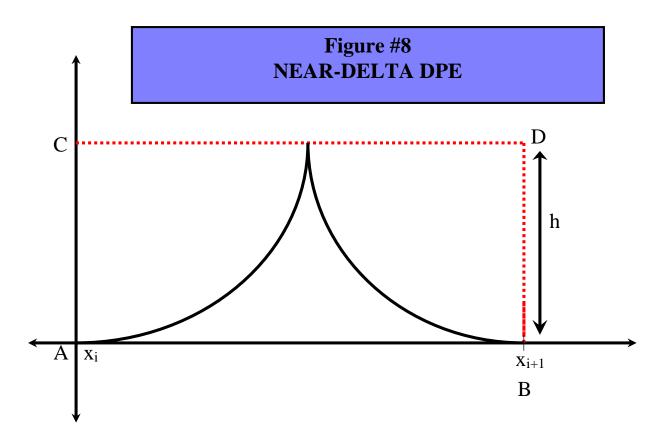




# Figure #6 PENALTY MINIMIZER METRIC - #2







## Figure #9 Monic B Spline Base Setup

