Overview of Data Fitting Component in Intel® Math Kernel Library (Intel® MKL)

Intel Corporation

Agenda

- 1D interpolation problem statement
- Computation flow
- Application areas
- Data fitting in Intel® MKL
- Data fitting API and usage model
- Data fitting performance
- Data fitting in applications

Optimization Notice

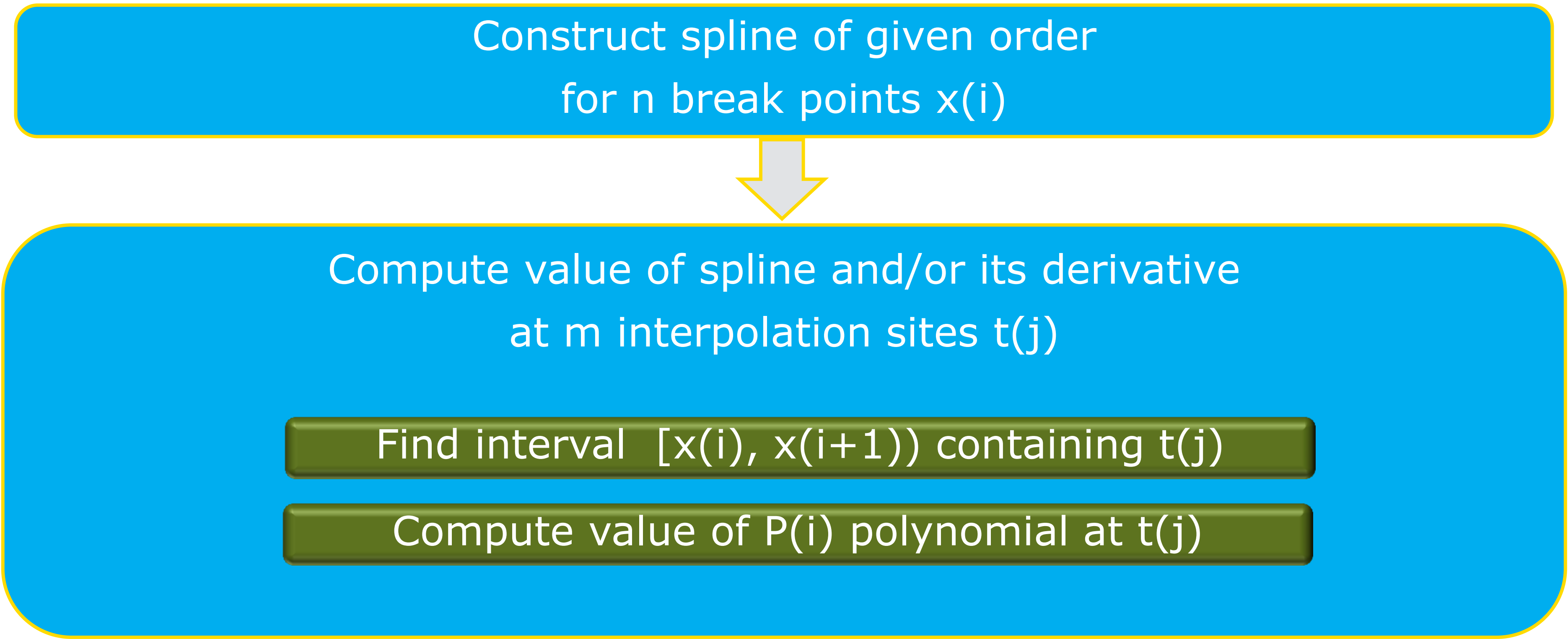
1D Interpolation Problem Statement

- For given table function {x(i), y(i)}, i=1,…,n
  - x(i): breakpoints in ascending order
  - y(i): values
- Approximate function f(x): f(x(i))=y(i)
- Evaluate value f(t(j)) and derivative f’ (t(j))
  - t(j), j=1,…,m: sites fall between or outside of interpolation interval [x(1),x(n)]
- Evaluate integral of f(x) over interval [a(j),b(j))
  - Integration limits a(j) and b(j) fall between or outside of interpolation interval [x(1),x(n)], j=1,…,m

Spline Based 1D Interpolation

- What is a spline?
  - Piecewise polynomial functions
  - g(x) := Pj(x), x belongs to [x(j), x(j+1))
  - Pj(x) - polynomial of degree k on the interval [x(j), x(j+1))
  - smooth up to order q at x(j) if derivatives up to order q for P(j-1) and Pj at x(j) exist and are equal
- Spline based methods are preferable over polynomial interpolation
  - Avoiding Runge’s phenomenon: Interpolation error increases when the order of the polynomial increases

Computation Flow



Construct spline of given order
for n break points x(i)

Compute value of spline and/or its derivative
at m interpolation sites t(j)

Find interval [x(i), x(i+1)) containing t(j)

Compute value of P(i) polynomial at t(j)

- **Integration has similar computational flow**
- **Cell search is the key building block**

Application Areas

- Data analysis and analytics
  - Approximation of statistical estimates like histogram
- Manufacturing
  - Geometrical modeling
  - *“B-spline recurrence relations … were used at Boeing, …, five hundred million times a day”* Carl de Boor, On Wings of Splines Newsletter of Institute for Mathematical Sciences, ISSUE 5 2004
- Energy
  - Surface approximation
- ISV
- Life sciences
  - Molecular dynamics simulation

Data Fitting in Intel® MKL

- Intel® MKL Data Fitting – SW solution for
  - Spline construction
  - Spline based interpolation and computation of derivatives
  - Spline based integration
  - Cell Search
- Current version of Intel® MKL supports 1-dimensional data fitting computations

Spline Construction and Boundary/Internal Conditions

Spline	Spline type
Linear	
Quadratic	Default, Subbotin
Cubic	Default, Natural, Hermite, Bessel, Akima
Look-up	
Stepwise constant	Continuous-right, Continuous-left
User-defined	

Boundary conditions	Internal conditions
Not-a-knot	1st derivative
Free-end	2nd derivative
1st derivative at the left/right endpoint	Knot array
2nd derivative at the left/right endpoint	
Periodic	
Function value at mid point of first cell	

Rich collection of splines that support different boundary or/and internal conditions

Interpolation, Extrapolation, and Integration

Feature	Comment
Computation of values, derivatives of arbitrary order	• Support of *a priori* information about structure of partition, and/or interpolation sites • In addition to default spline based interpolation library supports user-defined functions to • re-define default spline based computations on interpolation or/and extrapolation intervals • re-define cell search functions • Option to get results of cell search simultaneously with interpolation • User defined threading-friendly API
Computation of integrals	• Support of *a priori* info about structure of partition, and/or integration limits • In addition to default spline based interpolation library supports user-defined functions to • re-define default integration on interpolation or/and extrapolation intervals • re-define cell search functions • User defined threading-friendly API

Flexibility in support of various usage models for spline based computations

Optimization Notice

Cell Search

Feature	Comment
Computation of cell indices containing given sites	• Support of *a priori* information about structure of partition, and/or interpolation sites • In addition to default cell search computation library supports user-defined function to • re-define cell search functions • User defined threading-friendly API

Flexibility in support of various usage models for cell search

Data Fitting API and Usage Model

Step	Code example	Comment
Create a task	`status = dfdNewTask1D( &task, nx, x, xhint, ny, y, yhint );`	You can call the Data Fitting function several times to create multiple tasks
Modify the task parameters.	`status = dfdEditPPSpline1D( task, s_order, c_type, bc_type, bc, ic_type, ic, scoeff, scoeffhint );`	
Perform Data Fitting spline-based computations	`status = dfdInterpolate1D(task, estimate, method, nsite, site, sitehint, ndorder, dorder, datahint, r, rhint, cell );`	You may reiterate steps 2-3 as needed
Destroy the task or tasks	`status = dfDeleteTask( &task );`	

Cubic Spline Interpolation Example

- This example can also be found in the online Intel® MKL Reference Manual (link)

```
/* Initialize the partition and set their values */
. . .
. . .
/* Create a Data Fitting task */
status = dfdNewTask1D( &task, nx, x, xhint, ny, y, yhint );

/* Initialize spline parameters */
s_order = DF_PP_CUBIC; /* Spline is of the fourth order (cubic spline). */
s_type = DF_PP_BESSEL; /* Spline is of the Bessel cubic type. */

bc_type = DF_BC_NOT_A_KNOT; bc = NULL; /* Use not-a-knot boundary conditions */

/* Set spline parameters in the Data Fitting task */
status = dfdEditPPSpline1D( task, s_order, s_type, bc_type, bc, ic_type, ic, scoeff, scoeffhint );

/* Construct a cubic Bessel spline: */
status = dfdConstruct1D( task, DF_PP_SPLINE, DF_METHOD_STD );

/* Initialize interpolation parameters and set site values */
. . .
/* Compute the sline values at site(i), i=0,..., nsite-1 and place the results to array r */
status = dfdInterpolate1D(task, DF_INTERP, DF_METHOD_STD,nsite, site, sitehint, ndorder, &dorder,
                           datahint, r, rhint, cell );

/* De-allocate Data Fitting task resources */
status = dfdDeleteTask( &task );
```

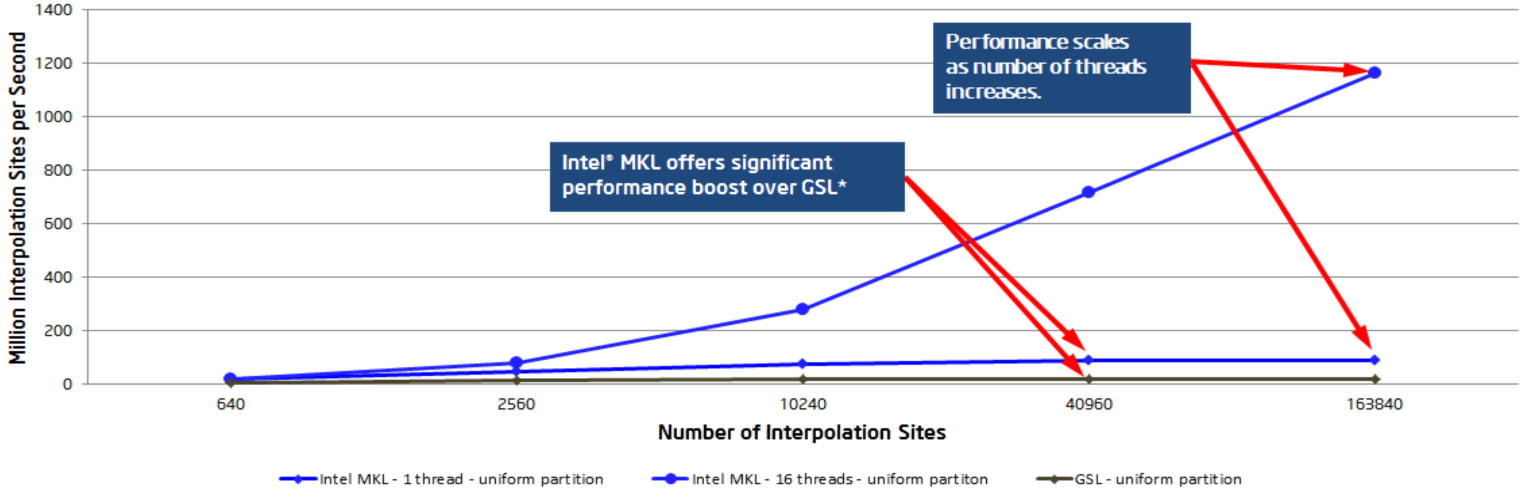
Cell Search Example

- This example can also be found in the online Intel® MKL Reference Manual (link)

```
/* Initialize a uniform partition */
. . .

/* Initialize function parameters; in cell search, function values are not necessary */
ny = 0;
y = NULL;
yhint = DF_NO_HINT;

/* Create a Data Fitting task */
status = dfdNewTask1D( &task, nx, x, xhint, ny, y, yhint );
. . .

/* Initialize interpolation (cell search) parameters */
nsite = NSITE;
/* Set sites in the ascending order */
. . .
sitehint = DF_SORTED_DATA; /* Sites are provided in the ascending order. */
datahint = DF_NO_APRIORI_INFO; /* No additional information about breakpoints/sites is provided.*/

/* Compute indices of the cells that contain interpolation sites.
   Results are stored in cell(i), i=0,...,nsite-1 */
status = dfSearchCell1D( task, DF_METHOD_STD, nsite, site, sitehint, datahint, cell );

/* Delete task and de-allocating resources */
status = dfDeleteTask( &task );
```

Data Fitting Performance: Interpolation

**Performance Improves using Intel® Math Kernel Library versus GSL*
Spline Construction and Interpolation on Intel® Xeon® E5-2600 Family Processor**



Performance scales as number of threads increases.

Intel® MKL offers significant performance boost over GSL*

Configuration Info - Versions: Intel® Math Kernel Library (Intel® MKL) 11.0; Hardware: Intel® Xeon® Processor E5-2690, 2 Eight-Core CPUs (20MB LLC, 2.9GHz), 32GB of RAM; Operating System: RHEL 6 GA x86_64; Benchmark Source: Intel Corporation.

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Construction of natural cubic spline with free end boundary conditions for function defined on uniform partition. Partition size is 1280. Spline-based values and first derivatives are computed.

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