SSJ User's Guide

Package `functionfit`

Function fit utilities

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This package provides basic facilities for curve fitting and interpolation with polynomials as, for example, least square fit and spline interpolation.

Contents

PolInterp

Represents a polynomial that interpolates through a set of points. More specifically, let $(x_0, y_0), \ldots, (x_n, y_n)$ be a set of points and $p(x)$ the constructed polynomial of degree n. Then, for $i = 0, \ldots, n$, $p(x_i) = y_i$.

```
package umontreal.iro.lecuyer.functionfit;
```

```
public class PolInterp extends Polynomial implements Serializable
```

Constructors

```
public PolInterp (double[] x, double[] y)
```

Constructs a new polynomial interpolating through the given points `(x[0], y[0]), ..., (x[n], y[n])`. This constructs a polynomial of degree `n` from `n+1` points.

Methods

```
public static double[] getCoefficients (double[] x, double[] y)
```

Computes and returns the coefficients the polynomial interpolating through the given points `(x[0], y[0]), ..., (x[n], y[n])`. This polynomial has degree `n` and there are `n+1` coefficients.

```
public double[] getX()
```

Returns the x coordinates of the interpolated points.

```
public double[] getY()
```

Returns the y coordinates of the interpolated points.

```
public static String toString (double[] x, double[] y)
```

Makes a string representation of a set of points.

```
public String toString()
```

Calls `toString(double[], double[])` with the associated points.

LeastSquares

Represents a polynomial obtained by the least squares method on a set of points. More specifically, let $(x_0, y_0), \ldots, (x_n, y_n)$ be a set of points and $p(x)$ the constructed polynomial of degree m. The constructed polynomial minimizes the square error

$$E^2 = \sum_{i=0}^{n} [y_i - p(x_i)]^2.$$

```
package umontreal.iro.lecuyer.functionfit;

public class LeastSquares extends Polynomial implements Serializable
```

Constructors

```
public LeastSquares (double[] x, double[] y, int degree)
```

Constructs a new least squares polynomial with points `(x[0], y[0]),..., (x[n], y[n])`. The constructed polynomial has degree `degree`.

Methods

```
public static double[] getCoefficients (double[] x, double[] y,
                                        int degree)
```

Computes and returns the coefficients of the fitting polynomial of degree `degree`. The coordinates of the given points are `(x[i], y[i])`.

```
public double[] getX()
```

Returns the x coordinates of the fitted points.

```
public double[] getY()
```

Returns the y coordinates of the fitted points.

```
public String toString()
```

Calls `toString` with the associated points.

BSpline

Represents a B-spline with control points at (X_i, Y_i). Let $\mathbf{P_i} = (X_i, Y_i)$, for $i = 0, \dots, n-1$, be a *control point* and let t_j, for $j = 0, \dots, m-1$ be a *knot*. A B-spline [1] of degree $p = m - n - 1$ is a parametric curve defined as

$$\mathbf{P(t)} = \sum_{i=0}^{n-1} N_{i,p}(t)\mathbf{P_i}, \text{ for } t_p \le t \le t_{m-p-1}.$$

Here,

$$N_{i,p}(t) = \frac{t - t_i}{t_{i+p} - t_i} N_{i,p-1}(t) + \frac{t_{i+p+1} - t}{t_{i+p+1} - t_{i+1}} N_{i+1,p-1}(t)$$

$$N_{i,0}(t) = \begin{cases} 1 & \text{for } t_i \le t \le t_{i+1}, \\ 0 & \text{elsewhere.} \end{cases}$$

This class provides methods to evaluate $\mathbf{P(t)} = (X(t), Y(t))$ at any value of t, for a B-spline of any degree $p \ge 1$. Note that the `evaluate` method of this class can be slow, since it uses a root finder to determine the value of t^* for which $X(t^*) = x$ before it computes $Y(t^*)$.

```
package umontreal.iro.lecuyer.functionfit;

public class BSpline implements MathFunction
```

Constructors

`public BSpline (final double[] x, final double[] y, final int degree)`

Constructs a new uniform B-spline of degree `degree` with control points at (`x[i]`, `y[i]`). The knots of the resulting B-spline are set uniformly from `x[0]` to `x[n-1]`.

`public BSpline (final double[] x, final double[] y, final double[] knots)`

Constructs a new uniform B-spline with control points at (`x[i]`, `y[i]`), and knot vector given by the array `knots`.

Methods

`public double[] getX()`

Returns the X_i coordinates for this spline.

`public double[] getY()`

Returns the Y_i coordinates for this spline.

`public double getMaxKnot()`

Returns the knot maximal value.

```
public double getMinKnot()
```

Returns the knot minimal value.

```
public double[] getKnots()
```

Returns an array containing the knot vector (t_0, t_{m-1}).

```
public static BSpline createInterpBSpline (double[] x, double[] y,
                                           int degree)
```

Returns a B-spline curve of degree `degree` interpolating the (x_i, y_i) points [1]. This method uses the uniformly spaced method for interpolating points with a B-spline curve, and a uniformed clamped knot vector, as described in `http://www.cs.mtu.edu/~shene/COURSES/cs3621/NOTES/`.

```
public static BSpline createApproxBSpline (double[] x, double[] y,
                                           int degree, int h)
```

Returns a B-spline curve of degree `degree` smoothing (x_i, y_i), for $i = 0, \ldots, n$ points. The precision depends on the parameter h: $1 \le$ `degree` $\le h < n$, which represents the number of control points used by the new B-spline curve, minimizing the quadratic error

$$L = \sum_{i=0}^{n} \left(\frac{Y_i - S_i(X_i)}{W_i} \right)^2 .$$

This method uses the uniformly spaced method for interpolating points with a B-spline curve and a uniformed clamped knot vector, as described in `http://www.cs.mtu.edu/~shene/COURSES/cs3621/NOTES/`.

```
public BSpline derivativeBSpline()
```

Returns the derivative B-spline object of the current variable. Using this function and the returned object, instead of the `derivative` method, is strongly recommended if one wants to compute many derivative values.

```
public BSpline derivativeBSpline (int i)
```

Returns the ith derivative B-spline object of the current variable; i must be less than the degree of the original B-spline. Using this function and the returned object, instead of the `derivative` method, is strongly recommended if one wants to compute many derivative values.

SmoothingCubicSpline

Represents a cubic spline with nodes at (x_i, y_i) computed with the smoothing cubic spline algorithm of Schoenberg [1, 2]. A smoothing cubic spline is made of $n+1$ cubic polynomials. The ith polynomial of such a spline, for $i = 1, \ldots, n-1$, is defined as $S_i(x)$ while the complete spline is defined as

$$S(x) = S_i(x), \qquad \text{for } x \in [x_{i-1}, x_i].$$

For $x < x_0$ and $x > x_{n-1}$, the spline is not precisely defined, but this class performs extrapolation by using S_0 and S_n linear polynomials. The algorithm which calculates the smoothing spline is a generalization of the algorithm for an interpolating spline. S_i is linked to S_{i+1} at x_{i+1} and keeps continuity properties for first and second derivatives at this point, therefore $S_i(x_{i+1}) = S_{i+1}(x_{i+1})$, $S'_i(x_{i+1}) = S'_{i+1}(x_{i+1})$ and $S''_i(x_{i+1}) = S''_{i+1}(x_{i+1})$.

The spline is computed with a smoothing parameter $\rho \in [0, 1]$ which represents its accuracy with respect to the initial (x_i, y_i) nodes. The smoothing spline minimizes

$$L = \rho \sum_{i=0}^{n-1} w_i \left(y_i - S_i(x_i)\right)^2 + (1-\rho) \int_{x_0}^{x_{n-1}} \left(S''(x)\right)^2 dx$$

In fact, by setting $\rho = 1$, we obtain the interpolating spline; and we obtain a linear function by setting $\rho = 0$. The weights $w_i > 0$, which default to 1, can be used to change the contribution of each point in the error term. A large value w_i will give a large weight to the ith point, so the spline will pass closer to it. Here is a small example that uses smoothing splines:

```
int n;
double[] X = new double[n];
double[] Y = new double[n];
// here, fill arrays X and Y with n data points (x_i, y_i)
// The points must be sorted with respect to x_i.

double rho = 0.1;
SmoothingCubicSpline fit = new SmoothingCubicSpline(X, Y, rho);

int m = 40;
double[] Xp = new double[m+1];       // Xp, Yp are spline points
double[] Yp = new double[m+1];
double h = (X[n-1] - X[0]) / m;      // step

for (int i = 0; i <= m; i++) {
   double z = X[0] + i * h;
   Xp[i] = z;
   Yp[i] = fit.evaluate(z);          // evaluate spline at z
}
```

```
package umontreal.iro.lecuyer.functionfit;
   import umontreal.iro.lecuyer.functions.*;
   import umontreal.iro.lecuyer.functions.Polynomial;


public class SmoothingCubicSpline implements MathFunction,
             MathFunctionWithFirstDerivative, MathFunctionWithDerivative,
             MathFunctionWithIntegral
```

Constructors

```
public SmoothingCubicSpline (double[] x, double[] y, double[] w,
                             double rho)
```

Constructs a spline with nodes at (x_i, y_i), with weights w_i and smoothing factor $\rho =$ `rho`. The x_i *must* be sorted in increasing order.

```
public SmoothingCubicSpline (double[] x, double[] y, double rho)
```

Constructs a spline with nodes at (x_i, y_i), with weights $= 1$ and smoothing factor $\rho =$ `rho`. The x_i *must* be sorted in increasing order.

Methods

```
public double evaluate (double z)
```

Evaluates and returns the value of the spline at z.

```
public double integral (double a, double b)
```

Evaluates and returns the value of the integral of the spline from a to b.

```
public double derivative (double z)
```

Evaluates and returns the value of the *first* derivative of the spline at z.

```
public double derivative (double z, int n)
```

Evaluates and returns the value of the n-th derivative of the spline at z.

```
public double[] getX()
```

Returns the x_i coordinates for this spline.

```
public double[] getY()
```

Returns the y_i coordinates for this spline.

```
public double[] getWeights()
```

Returns the weights of the points.

```
public double getRho()
```

Returns the smoothing factor used to construct the spline.

```
public Polynomial[] getSplinePolynomials()
```

Returns a table containing all fitting polynomials.

`public int getFitPolynomialIndex (double x)`

Returns the index of P, the `Polynomial` instance used to evaluate x, in an `ArrayList` table instance returned by `getSplinePolynomials()`. This index k gives also the interval in table $\mathbf{X}$ which contains the value x (i.e. such that $x_k < x \leq x_{k+1}$).

References

[1] C. de Boor. *A Practical Guide to Splines*. Number 27 in Applied Mathematical Sciences Series. Springer-Verlag, New York, 1978.

[2] D. S. G. Pollock. Smoothing with cubic splines. Technical report, University of London, Queen Mary and Westfield College, London, 1993.