1-d and n-d Functions

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1-d Function Hierarchy

Function1D Base Class

- standard interface of 1-d functions.
- eval(), $f(x)$, $f'(x)$ and $f''(x)$
- integral(), $\int_a^b f(x)dx$
- option to use finite difference and Gaussian quadrature.

1-d Function Hierarchy (continued)

Piecewise Functions

- derived from Function1D
- piecewise constant
- piecewise linear (continuous)
- piecewise linear (non-continuous)
- B-spline

1-d Function Hierarchy (continued)

Chebyshev Approximation

- derived from Function1D
- linear combination of Chebyshev basis polynomials
- smooth
- 'mini-max' property

n-d Function Hierarchy

FunctionND Base Class

- standard interface of n-d functions.
- eval(), $f(\mathbf{x})$, $\nabla f(\mathbf{x})$ and $\nabla^2 f(\mathbf{x})$
- integral(), $\int\int f(\mathbf{x}) d\mathbf{x}$
- option to use finite difference to compute gradient and Hessian.

n-d Function Hierarchy (continued)

2-d Piecewise Functions

- derived from FunctionND but specific for 2-d.
- piecewise constant
- B-spline surface (tensor product of B-spline basis)
- bilinear surface (special case of B-spline, special handling)

n-d Function Hierarchy (continued)

Chebyshev Surface

- derived from FunctionND but specific for 2-d.
- tensor product of Chebyshev basis polynomials.
- nice properties due to Chebyshev basis polynomials.

1-d and n-d Functions (extended)

Client Functions

- derived from the common base classes, client supplied implementation.
- accepted anywhere in the library as 1-d or n-d functionals, i.e. root finding, optimization, etc.

Vector-valued Functions

VtrValueFunctionND

- base class as common interface
- $\mathbf{y} = F(\mathbf{x})$, $\mathbf{y}$ is $m \times 1$ and $\mathbf{x}$ is $n \times 1$.
- client supplies implmentation to compute $\mathbf{y}$ and Jacobian $\mathbf{J}$.
- option to use finite difference to compute $\mathbf{J}$.
- mostly used for model calibration.

1-d Interpolation (generalized)

Cubic B-spline as Basis

- beyond natural or clamped spline, or Hermite interpolation polynomial.
- match any combination of $f(x_i)$, $f'(x_i)$ and $f''(x_i)$ at given data point x_i.
- automatic placement of B-spline knot points.

1-d Integration

Quadrature in General

- $\int_a^b f(x)dx = \sum_{k=0}^n w_k f(x_k)$, $w_k = \int_a^b L_{n,k}(x)dx$, $L_{n,k}(x)$ is Lagrangian basis polynomial of degree n.
- trick is to partition $[a, b]$ to quadrature data points $\{x_k\}, k = 0, \cdots, n$.

Adaptive Gaussian Quadrature

- better than Newton-Cotes family methods, i.e. trapezoidal, Simpson.
- better than composite Newton-Cotes methods or Romberg method in the sense of optimal placement of x_k.
- ensure accuracy in each sub interval, more points are placed if curvature dramatically changes.

1-d Root Finding

Root Finding In General

- bisection, Brent: guaranteed convergence but not so great on convergence rate.
- Newton: require $f'(x)$, sencond order convergence rate, but not guaranteed to converge if x is far from solution x^*.
- Secant: same idea as Newton but approximate $f'(x)$, superlinear rate, convergence not guaranteed.

Safeguared Newton

- combine the idea of Newton method with bisection.
- bracketing on the fly of trial Newton steps.
- tests based on fixed point iteration theorem: OK $\rightarrow$ Newton mode, otherwise $\rightarrow$ bisection mode.
- Newton mode: if $f'(x)$ available, classic Newton step update, otherwise, predict from rational polynomial interpolation.

1-d Minization

Safeguarded Quadratic Approximation

- combine Golden section search with quadratic approximation.
- guaranteed convergence and second order convergence rate if x is close to solution x^*.
- initial bracketing mode and subsequent safeguarded mode.
- if $f'(x)$ is available, evaluation at two points to construct the approximation, otherwise, evaluation at three points.

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