A CATALOG OF ALGORITHMS FOR APPROXIMATION

ERIC GROSSE
AT&T BELL LABORATORIES

Abstract. This is an outline and a list of algorithms for numerical approximation, with references to the literature and pointers to available code. The database has been formatted here as an indented tree using TEX; alternatively, it may be viewed in graphical form or may be traversed using a C program or a World Wide Web browser.

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Key Words. approximation algorithms, bibliography, database, library routines, subroutines, numerical consultant, netlib, walk

1. Introduction. There is a large gap between the classical polynomial, rational, and univariate spline fitting taught in textbooks and the variety of additional methods that have been developed for complicated real-world problems. Someday we may hope for a Knuth to write the definitive survey, but probably it is too soon for that. The following categorized list of algorithms can help bridge this gap in the meantime. This catalog is designed first to assist in numerical analysis consulting; second, to guide the acquisition of software for netlib[243]; and third, to help inventors of new methods search for prior art.

Notes in square brackets in the bibliography indicate where software may be found. Most commonly this will be a directory in netlib or one of the standard commercial libraries[27, 438, 559, 299]. For example, to get LSQR[571], send the one-line message `send lsqr from misc` by electronic mail to `netlib@research.att.com` or `research!netlib`. The name "toms" refers to the Collected Algorithms of the ACM, available via IMSL and netlib. A server `statlib@temper.stat.cmu.edu`, spun off from netlib to serve the statistical community, also contains interesting algorithms.

When known, references most closely related to final code are given. These will often not be the primary reference for the idea and hence many classic papers in approximation do not appear. Analytical papers are cited if they provide useful guidance on choosing between codes or if the topic seems ripe for computation although no algorithmic papers are known. Generally the comparative foundations do not exist for recommending a best method in each category. It would have been desirable to mention only methods for which convincing numerical evidence has been reported. Consistently adhering to such a policy would have made a very much shorter list but would necessarily have left out many good algorithms. Where NAG routines are apparently superseded by DASL routines, they have not been listed. Methods requiring an (expensive) software license have been de-emphasized, particularly when competitive public versions are available. Finally, it was not feasible to cite the papers in this proceedings; but they report a number of exciting developments and the reader who has not already done so is encouraged to look at the rest of the book!

2. Classification. In addition to the traditional characterization of practical approximation as fundamentally a choice of *form* and *norm*, this scheme adds a third category, *variable*, to reflect the important choices of sample designs and coordinate transforms. The primary classification is by form since it corresponds most directly to the literature. Some methods are not specific to a particular basis but are more readily characterized by, for example, the norm they optimize; these are listed under norm.

Another possible characterization would have been by the operation involved. Some of these are: evaluate, differentiate, integrate; interpolate, extrapolate, local fit; best or good fit in various norms; diagnostics, error estimation; conversions between different bases; i/o, graphics; zeros, maxima, other critical features.

The database is formatted below as an indented tree with cross-links. The bracketed numbers at the leaf nodes are lists of references. While this paper snapshot may be convenient for distribution, interactive software providing easier use is described in section 3.

form (basis of approximating space)
- polynomial, rational
  - real polynomial
    - power
      - evaluation [400, 284, 777, 666, 395]
      - integrals [666]
    - Newton form of interpolating polynomial [331, 262, 286]
    - Chebyshev
      - interpolation to function and derivative data [471]
      - least squares [184]
      - evaluation [323, 299, 27, 98]
      - derivatives [27]
      - integrals [27]
      - standard errors from least squares fit [27]
      - endpoint constrained [473]
    - `Bezier` barycentric, Bernstein-Bezier curves and patches [411, 356, 276, 276, 647, 672, 666, 676]
      - `deglower` degree lowering [186, 429, 259]
    - general orthogonal [295, 757, 299, 679, 176, 723, 334]
      - adding and deleting points [210, 266]
      - Sobolev norm [440]
    - `polycon` constrained [164, 518, 461]
    - multivariate
      - evaluation [139]
      - approximation, interpolation [160, 331, 128, 57, 251, 543, 461, 596]
  - real rational [727, 460, 641, 506, 218, 590]
    - `Remez` Remez exchange [502, 529, 119, 144, 446]
      - Remez, first (single exchange) [248, 561]
      - Remez, second (multiple exchange) [191, 691, 149, 56, 151]
    - `diffcor` differential correction [299, 458, 149]
    - linear inequality method [480, 249]
    - interpolation [370, 371, 193, 195, 194, 734]
      - barycentric [82, 83]
    - Padé [404, 517, 195, 728]
    - power of polynomial in denominator [140, 250]
  - complex polynomial, rational [702, 750, 752]
    - polynomial [294, 607, 389, 286, 710]
    - rational [609, 727]
  - zeros of polynomials [578, 500, 441]
- spline, finite element
  - `crease` discontinuities (jump, crease, edges)
    - known, fixed crease [99, 305, 682, 245]
    - unknown crease, to be found [546, 682, 522, 132, 724, 77, 484, 483, 339]
  - splines
    - univariate
      - piecewise linear
        - tabulate at arguments where values need few digits [327, 3, 708, 513, 328, 778]
        - `segment` breakpoint placement [434, 575, 760, 573, 744, 245, 527]
      - pch: piecewise cubic Hermite [317, 316]
        - `u-der` derivative estimation [5, 267, 437, 8]
      - pp: general piecewise polynomial [562]

  - almost smooth (jumps less than ϵ)
    - (no citations at hand, though surely some exist)
  - evaluation of general piecewise polynomial [101, 438]
  - one-pass least squares fitting [774]
- B-splines [101]
  - fitting, interpolation
    - interpolation [101, 27, 438]
      - `optinterp` "optimal" spline interpolation [101, 438, 326, 716]
      - many-knot interpolation [204]
    - end conditions for interpolation [495, 66]
    - local, variation diminishing [499, 204]
    - quasi-interpolation [101, 639, 158]
    - least squares fitting
      - fitting discrete data [101, 27, 438, 299]
      - fitting user function [299]
    - l_1 fitting to data points [187]
    - l_∞ fitting to a function [560, 91]
  - evaluation, derivatives, integral
    - spline evaluation [101, 27, 438, 299, 487, 689]
    - B-spline basis evaluation [101, 299]
    - spline derivatives [101, 27, 438, 299]
    - B-spline basis derivatives [101, 299]
    - spline integrals [27, 438, 299, 325]
    - B-spline basis integrals [299, 740]
    - Fourier transform [333, 388, 548, 390, 221]
    - `knotins` knot insertion and degree raising [173, 92, 476, 93, 199, 94, 498]
  - `B-spline-zero` zeros [235, 369]
  - subdivision, knot insertion →**`knotins`**
  - degree raising [593, 174, 498]
    - degree lowering →**`deglower`**
  - `B-diag` diagnostics, error estimation
    - standard errors from least squares fit [27]
    - function and spline [299]
    - two splines [299]
  - rational B-splines [583, 488]
- Bernstein-Bezier curves →**`Bezier`**
- conversion between different bases [101, 313, 429, 349, 315, 722]
- specialized splines [642]
  - elastica [486, 504, 611, 351, 455, 124, 451, 125, 261]
  - `nu-spline` ν, β, γ, Manning, Farin, W-F [550, 313, 421, 290, 315, 291]
  - taut splines, splines under tension [697, 167, 101, 617, 555, 613, 646, 468, 615]
  - `network` minimum norm network spline [553, 555, 556, 540]
  - weighted splines [644, 290, 472]
  - other [664, 25]
    - Catmull-Rom [141, 54]
    - discrete spline [252, 173]
    - EHB-spline (unusual smoothness constraints) [444]
    - `spec-spline` spectral spline [379]
    - conic spline [574, 591, 582]
    - Bernoulli spline [699]

- `adaptive` free knots [28]
  - `refine` refinement
    - refine intervals with large residual [235, 187, 2, 539]
    - refine triangle [659]
    - refine using critical features [648]
    - segmented piecewise linear approximation →`segment`
    - k-d tree [310, 626, 166, 380, 311]
    - hierarchical rectangular grid [620, 105, 198, 40]
      - hierarchical basis [775, 21]
        - `wavelet` wavelet, quadrature mirror filter [383, 84, 739, 532, 156]
      - quadtree, octree [772]
      - rectangular covering [74, 377, 75]
    - recursive subdivision [470, 255, 533, 426, 637]
      - knot insertion for splines →`knotins`
      - `bounds` bounds [360, 150]
  - free knots [104, 585, 453, 53, 562, 560]
    - de Boor newnot [100, 661, 438, 598]
    - methods applied to differential equations [577, 758, 464, 134, 32]
  - free knots for piecewise constant [269]
  - free grid in more than one variable [216]
  - nonuniform sampling to ameliorate aliasing [538]
  - quasirandom (more uniform than true random would be) [651, 298]

- multivariate
  - pp: general piecewise polynomial [14, 342]
    - Bernstein-Bezier patches →`Bezier`
  - `tensor` tensor product splines [576, 102]
    - fitting, interpolation
      - interpolation [101, 27, 756]
      - least squares fitting [130, 403, 227, 382, 229, 27]
      - low rank [222, 311]
    - twist estimation [276]
    - evaluation, derivatives
      - evaluation [27, 438, 299]
      - derivatives [27, 438]
      - integrals [438]
  - `plate` thin plate splines [121, 99, 302, 303, 481, 62, 599, 732, 686]
    - polyharmonic spline [601, 534, 602, 603]
  - simplex splines [205, 206, 425, 366, 343, 345, 368]
  - box splines; uniform grid [639, 94, 200, 442, 390, 201]
    - evaluation [426, 155, 474]
    - interpolation and quasi-interpolation [158, 157, 196, 756, 445]
  - triangular B-spline [307, 676, 94, 293]
  - super spline [159, 667]
  - minimum norm network spline →`network`
  - conversion between different bases; degree lowering [432]

- `fem` finite elements [161, 72, 457]
  - bivariate
    - triangle
      - quadratic, piecewise quadratic [586, 588, 687, 237]
      - cubic, piecewise cubic [344, 367]

Hsieh-Clough-Tocher C^1 cubic macro-triangle [169, 81, 80, 509, 275, 767]
C^1 quintic, piecewise quintic [80, 596]
rational [524, 44, 510, 745, 16, 416]
other [552, 685, 596]
rectangle [530, 59, 557]
`iso` isoparametric approximation ($\min_{P,Q} \|f \circ P - Q\|$) [362, 509, 308, 283, 162]
`param/irr` irregular patches for otherwise rectangular grid [635, 700, 493, 579]
trivariate and general dimension [638]
tetrahedron [10, 11, 767, 769, 629]
`blendmult` discretizations of blending on simplices [508, 49, 13, 374]
`est+fem` estimate nodal information for finite element
`triang` triangulation [63]
Delaunay-Thiessen (dual to Voronoi polygons); max-min angle [563]
bivariate [478, 6, 168, 49, 297, 296, 260]
three and more [110, 748, 449]
other (data-independent) triangulation criteria
min-max angle [754]
data dependent triangulation [257, 600, 669]
searching general triangulation for given point [478, 666, 594]
dealing with nonconvex domains [645]
estimate values, derivatives (for use with finite element)
univariate →`u-der`
least squares local quadratic [478]
weighted average of directional derivatives [6, 510, 7, 49]
variational method (minimize integral of derivatives) [12]
minimum norm network →`network`
finite element →`fem`
`blending` blending
rectangular patch [142, 46, 44, 73]
triangular patch [45, 44, 373, 551, 552, 16, 391, 288]
`blendcur` network of curves [763, 443]
`recontour` slices parallel to coordinate plane [321, 97, 466]
`Urysohn` Urysohn's lemma [143]
more than two variables →`blendmult`
boundary data as basis functions [719]
`blendpt` experimental design [361, 220]
other specific approximating spaces
trigonometric [392, 299, 340, 113, 253]
FFT [177, 692, 715, 240, 707, 684, 714, 197]
spectral methods [364, 365, 133]
special functions (approximation by, not approximation of)
`exp` sum of exponentials [392, 456, 630, 749, 694, 751]
`varp` VARPRO [353, 462, 463, 352, 299]
`gaus` sum of gaussians [652]
sinc [698, 129, 83]
kernel smoothing [170]
moving least squares
distance weighted interpolation (Shepard) [681, 363, 44, 304, 491, 280, 50, 614]
(finite weight) least squares [523, 165, 475, 522, 166]
radial basis functions

Hardy's multiquadrics [399, 301, 289, 587, 68, 67]
thin plate splines $r^2 \log r^2$ →`plate`
sum of gaussians →`gaus`
algorithms applicable to many radial bases [254, 256, 123, 526, 445, 693]
other [634]
wavelet, quadrature mirror filter →`wavelet`
Urysohn's lemma →`Urysohn`
grid refinement →`refine`
techniques for combining specific methods
directrix, correspondence, and generator [633, 35]
extension of univariate methods to multivariate
tensor product and similar methods
rectangular grid data; tensor splines →`tensor`
slices parallel to coordinate axis [164, 27]
scattered data [409]
missing data : $\Delta u = 0$
curved mesh lines [185]
rational product [459, 413]
blending, Coons patch, transfinite element →`blending`
additive $f(x, y) \approx g(x) + h(y)$ [410, 149, 408, 569, 311, 743]
nomographic $\approx f(u(x) + b(y))$, ACE [149, 116]
projection pursuit, $\approx \sum f(\alpha \cdot x)$ [312, 718]
multistage methods
estimate nodal information for finite element →`est+fem`
interpolate scattered data onto rectangular grid [663]
Boolean sum, other than blending [47, 44, 475]
smooth averaging of overlapping local patches [519, 452, 300, 731, 302, 207, 26]
iterated fitting of residual [312, 287, 636]
Ivakhnenko GMDH [277]
adaptive learning networks [123]
isoparametric approximation ($\min_{P,Q} \|f \circ P - Q\|$) →`iso`
generalized cone [549]
offset [143, 633, 278]
fillets [424, 747, 592, 624, 633]
parametric, geometric/visual continuity
parametric smoothness desired [27]
curves
`vparam` choice of parameterization variable [268, 511, 313, 430, 485, 276, 278, 18]
`tl2` orthogonal distance regression splines [735, 406, 96, 512, 721]
ordering scattered points [217]
spline [235]
piecewise conic [525, 309, 527, 431]
surfaces [152]
irregular patches for otherwise rectangular grid →`param/irr`
only geometric smoothness of locus of points needed
curves [103, 357, 649, 472, 477, 677, 218]
ν, β, γ, Manning, Farin, Wilson-Fowler splines →`nu-spline`
surfaces [274, 442, 554, 683, 659, 616]
abstract spaces
Haar system [213]

sum of exponentials →**exp**
Remez exchange →**Remez**
generating function methods (generalized Padé) [694]
linalg general linear basis functions
driver routine for user-supplied linear basis [27, 438]
kernel code [242]
linear equations [337, 354, 246, 101]
Linpack [244, 175]
solving Vandermonde systems [88, 329, 87, 712, 417, 418, 58, 131]
least squares [42]
unconstrained [210, 571, 29, 145, 86, 420, 85]
constrained [405, 347, 736, 397, 163, 43]
least p-norm [215]
opt general non-linear basis functions [117, 224, 376, 225]
separable nonlinear least squares →**varp**
zeros of splines →**B-spline-zero**
implicit algebraic equations [348, 747, 592, 675, 37, 36]
patches on quadric surfaces [746, 238]
patches on cubic surfaces [492]
approximation of parametric curve by implicit [572, 154, 584]
approximation of implicit curve by parametric [542]
paramdat data near parametric curve
near circle or ellipse [95, 78, 188, 628]
differential equations [737]
functional approximation [535, 531]
norm (criteria of approximation, figure of merit, nonstandard data)
classical L_p and analogous norms
l_2 [350]
total least squares, orthogonal distance regression →**tl2**
l_∞, L_∞ [447, 752]
Remez exchange →**Remez**
approximation by l_2 solution [608]
overdetermined linear system [51, 115, 702, 701]
underdetermined linear system [717]
differential correction →**diffcor**
Hankel norm ("CF" or "AAK" approximation) [727, 641]
l_1 [1, 52, 55, 187]
piecewise smooth [501]
sum of norms [570, 387]
Hausdorff $\max[\max_{y\in G}\min_{x\in F}||x-y||, \max_{y\in F}\min_{x\in G}||x-y||]$ [678]
statistically motivated metrics
maximum likelihood [223, 713, 568, 126]
AIC (Akaike's Information Criterion) [4, 619, 33]
Markov random field [336, 515]
bounding the relative error [660, 597]
measures of convergence [638]
penalties, smoothing, tolerances
choosing weights in l_2 and other norms [764, 718]
app-curv weighted norm of second derivative to approximate curvature [644, 245]
$l_2 + penalty$

- L_2 norm of first derivative, "minimum length" [39, 440]
- L_2 norm of high derivative [414, 415, 101, 438]
- l_2 and jumps in high derivative [230]
- jumps in divided difference [759]
- choice of smoothing parameter [585, 619, 605, 396]
  - **GCV** generalized cross validation [338, 226]
    - univariate [741, 567, 435, 765, 427, 469, 671]
    - bivariate [62, 771]
- weighted norm of second derivative to approximate curvature →`app-curv`
- energy of thin plate [599]

min $\int g''^2$ subject to $|g(t_i) - z_i| \le \epsilon$ [733]

divided differences as a measure of noise [190]

interpolation [326]
- at Chebyshev points [621, 411]

fair, pleasing [76, 528]

constraints
- periodic [496, 522, 604, 235, 680, 699]
- monotone, comonotone [138]
  - quadratic [627, 665, 70, 358]
  - cubic [318, 178, 436, 239, 738, 212, 208]
    - $O(h^4)$ [263, 770, 69, 332]
  - rational quadratic [219, 656]
  - bivariate [70, 183, 136, 137, 180, 732, 203, 658]
  - monotone, other forms or general order [106, 183, 642, 613, 187, 606]
- convex
  - quadratic [520, 627, 64, 358]
  - cubic [101, 653, 654]
  - with penalty term for smoothing [439, 23, 265]
  - convex, other forms [547, 228, 147, 673, 179, 613, 187, 282, 202, 658]
- one-sided, non-negative [630, 65, 564, 656, 657, 566, 208]
- specialized constraints [566]
  - **branch** branching [690]
  - integer [381]
  - specific to polynomials →`polycon`
  - "essentially non-oscillatory", "total variation diminishing" [375, 402, 401, 776]
  - ellipticity $\partial_{12}^2 \le \partial_{11}\partial_{22}$ [192]
  - cusp, inflection, self-intersection [258, 507]
- abstract methods [536]
  - semi-infinite programming [630, 341, 109, 710, 285]

data nonstandard data
- cross sections [236, 490, 346, 668, 264, 61]
  - blending methods →`recontour`
- given Fourier series coefficients, as in crystallography
  - rational in cos, sin [148]
  - spectral spline →`spec-spline`
- derivative data
  - given gradients, get surface; "shape from shading" [428, 482, 181]
  - given only gradient directions [209]
  - potential, stream function [742, 20]
- integral data

      - given integrals over small subintervals [60, 643, 655]
      - given flux, get velocities [394]
      - given moments [319, 320, 640]
    - missing data [718]
  - bounds →`bounds`
  - multiple scales or resolutions [132, 77]
- variable (coordinate transform, mesh generation)
  - geometry of the domain or graph
    - data on rectangular grid →`tensor`
    - data on nearly rectangular grid [636]
      - irregular patches for otherwise rectangular grid →`param/irr`
    - data along tracks, possibly intersecting [270]
      - blending on network of curves →`blendcur`
    - infinite interval [460]
    - functions defined over the surface of a sphere
      - tensor grid (latitude, longitude) [705, 706, 742, 231, 233, 234, 346, 725, 670]
      - uniform triangulation [63, 281]
      - scattered over sphere [479, 612, 34, 170, 292]
      - curves on the surface of a sphere in 3 or 4 dimensions [247, 556, 622]
    - branching curve; multivalued function →`branch`
    - points lying near a parametric curve →`paramdat`
    - projective space [489]
  - nonstandard data →`data`
  - discontinuities (jump, crease, edges) →`crease`
  - experimental design [537, 107, 286]
    - sample at Chebyshev points $\cos \frac{j\pi}{n}$ [423]
    - optimal statistical design [111, 273, 398]
    - blending →`blendpt`
  - coordinate transformation [729, 758, 720, 116]
    - scaling, centering, sphere-ing, decorrelation [730, 31]
    - conformal mapping [726, 412, 90]
    - polar coordinates [232]
  - selection of regression variables [311]
    - stepwise [505, 324, 359]
    - all subsets [422, 30]
  - choice of parameterization variable →`vparam`
  - isoparametric finite elements →`iso`
  - mesh generation, refinement
    - simple spline mesh utilities [101, 27, 299, 438]
    - "optimal" spline interpolation (particular choice of knots) →`optinterp`
    - segmented piecewise linear approximation →`segment`
    - stopping criteria for grid points
      - plateau in $||r||$ [101]
      - $\text{autocorr}(r) \leq 1/\sqrt{2(N-1)}$ [585]
      - cross-validation →`GCV`
      - maximum likelihood [114]
    - triangulation, given scattered points →`triang`
    - adaptive grids →`adaptive`
    - multivariate mesh generation [720, 448, 457, 38, 79, 454, 526, 631]
  - file format [153, 182, 494, 589]

boundary data structures [755, 766, 762, 9]
diagnostics
recognizing noise [385, 565]
recognizing outliers and influential points [674, 503]
recognizing redundancy [384]
diagnostics specific to B-splines →`B-diag`
diagnostic graphics [505, 729, 17, 71, 407]
contouring [632]
irregular grid [514, 99, 634, 650, 595, 211, 768]
rectangular grid [523, 703, 696, 662, 704, 687, 779]
higher order than quadratic; general functions [272, 372]
contour surfaces for function of three variables [153, 279, 580, 623]
color spectrum generation [378]
tests, benchmarks
standard test datasets [5, 585, 523, 478, 6, 318, 301, 305, 17, 661, 314, 419]
test methodology [189]
programs to test approximation algorithms [172, 709]
evaluations of algorithms [301]
tools from other fields
linear algebra →`linalg`
multigrid [521, 122]
optimization →`opt`
continuation, homotopy, surface-surface intersection [618, 753, 497]
surface-surface intersection methods [127]
arithmetic
multiple precision [118, 695]
interval [541]
basic arithmetic and special functions [773, 610, 625]
optimization and zero-finding [335, 465]
random number generators [467, 516, 298, 386, 19, 22, 581]
omitted topics
time series, digital filters, signal processing [240, 108, 761, 450]
finding intersections [112, 241, 433, 348, 146, 154, 558, 545, 544]
minimal surfaces [41]
quadrature [355, 214, 48]
special functions [400, 172, 171, 323, 322, 708, 711, 98]
elliptic integrals, Jacobian elliptic functions [271, 135]
extrapolation, acceleration of series [89, 120, 688]

3. Software for examining the catalog. The listing above is an adequate but hardly convenient way to look at the catalog. An interactive program for walking over the tree (actually, directed graph) is clearly preferable. Publicly available menu systems of this sort exist, but require numeric node labels and a specialized editor. Having mouse-based cut-and-paste, regular expression searching, undo, multiple windows, automatic backup against system crash, and other such features common to modern editors makes specialized editors unattractive. Instead I wrote my own menu system in one evening, a cost quite insignificant compared to typing in the database, which itself is insignificant compared to reading all those papers!

More recently, the database has been converted to an HTML file, `ftp://netlib.att.com/netlib/a/catalog.html.Z`, for use by World Wide Web browsers.

For those who nevertheless prefer paper, a PostScript copy of the catalogue is available from `netlib@research.att.com` by the request `send catalog from research/nam`.

Particularly when building a large graph with many cross links, it can be helpful to see a graphical representation of the walk database. There is an option to produce input for `dag`[330].

Another option produces a file which can be loaded into Hypercard. In order to fit onto the small Macintosh screen, there are a maximum of eight alternatives at any node. This might not be such a bad choice on psychological grounds as well. In one detail these interactive programs supply a bit more information than the typeset version; in place of the numeric reference number is a brief note that may indicate a particular routine or hint at important ideas of the algorithm not obvious from the title.

Keyword search is possible, though the database wasn't really designed with this in mind. To do a search via `netlib`, send a message of the form `find Schumaker in approximation`. "Schumaker" may be replaced here by any other pattern to be matched against the BibTEX database using the Unix system command egrep.

A weakness of the current system for some users is the absence of a glossary. Faced with a difficult choice at some point in walking the tree, it might be useful to look at the precise definition of terms.

End users would prefer everything to be indexed under "problem" instead of "form" and "norm", but that will take a lot more thought. The present catalog is to such an expert system as the Merck manual is to the Mycin program. The following short list hints at some of the relevant questions such a consultant would ask the user.

- given data
  - arrangement of data
  - range of variables
- criteria and constraints
  - norm, weights
  - continuity class (C^k or G^k) of fitted surface with respect to
  - point of evaluation
  - data ordinates
  - data abscissae
- periodic
- shape fidelity (monotone, convex, "fair")
- local or global dependence on data
- other constraints
- how approximation is to be used
  - values, derivatives, integral, plotting, extrapolation
- expected characteristics of data
  - singularities or peaks
- other considerations
  - desired form; interpreting coefficients
  - rotational, affine invariance in abscissae; linearity in ordinates
  - speed, memory
  - polynomial precision order, asymptotic convergence rate
  - sensitivity to noise in data, rounding error
  - failure modes
  - available libraries, languages

In some ways it would be more natural to classify the methods independently along several axes. But with so many methods, this would be awkward to display and traverse. A more classical expert system using production rules could probably handle this, but history suggests the result would be unreadable by others and hence not susceptible to peer review.

TABLE 1
`warmup` *attributes for Port.*

attribute	values
form	rational; spline; Bspline
op	fit; eval; deriv; int; errest; mesh
dat	function; spline; accurate; noisy
shape	wiggles-allowed; monotone-in,monotone-out
dorder	values; derivatives; integral
spacing	uniform; piecewise-uniform; multiplicities

A partial solution is provided by the program `warmup`, which takes a list of routines with associated attributes and automatically builds a decision tree in the form of a `walk` database. The attributes used for describing approximation routines in the Port library are shown in Table 1. Using only these values, `warmup` reproduced practically the same `walk` tree that was created manually by Norm Schryer.

This strategy is motivated by my observation of typical consulting at Bell Labs. A physicist walks into my office and gives me about five sentences describing her problem before I interrupt with a few questions and offer a possible algorithm. The point is that she will naturally mention half a dozen attributes that drastically narrow the range of possibilities. If this is not the first time we have talked, I probably remember from previous sessions various attributes she prefers in a code. `Warmup` appears well suited to this mode, if we can ever get an English language front end that can translate from physics into numerical analysis jargon. Various attributes would be recognized as either required, prohibited, or irrelevant; restricting the database according to this user profile yields a small decision tree by a greedy algorithm of picking for the next decision that attribute that minimizes the depth of the resulting subtrees.

4. Disclaimers. This is a catalog of a diverse collection, as distinguished from a table of contents of a high-quality mathematical software library. Certainly it would be pleasant if all routines adopted compatible calling styles, names, and data representations. But users see lots of interfaces anyway because they use collections of libraries. The enormous effort of making systematized interfaces means that libraries tend to fall behind the research front. Finally, even well-tested library routines may still have subtle numerical problems. Certainly the commercial libraries are valuable and well worth the rental. Library authors often do a much better job than the typical researcher when it comes to providing good example programs, carefully checking user input, and worrying about error messages. But there is also a place for research codes in exotic applications and to gain experience with different algorithms, in order to know what ought to go next into the libraries. Traditionally the time and expense of acquiring such research codes has been a major impediment, but netlib offers a solution. Moreover, programming environments have improved so much that coding up a method straight from a well-written article is often easy. Still, it should be clearly understood that research codes must be used with the same professional caution you would want your doctor to exercise when trying a new procedure.

Another worthwhile project would be to collect and standardize test problems, as David Gay has done for linear programming in `netlib/lp/data` and Chris Fraley has done for unconstrained optimization in `netlib/uncon/data`. Gay found that it was best to compress the files and distribute C and Fortran programs for unpacking them into the standard MPS file format. Some places to start would be [5][585][523][478][6][318][301][305][17][314] [419]. I would be willing to contribute an example coming from an important application in VLSI, monotone fitting of current as a function of the three independent terminal voltages for a MOSFET transistor [183].

Comments are welcome and will be incorporated in the online edition of the catalog. Send electronic mail to `ehg@research.att.com` or `uunet!research!ehg`. As well as pointing out missing papers, please note defects in the citations; in a list of this size, an inadequately classified paper is as good as lost. Since the list will always be incomplete, anyone seriously concerned with a particular topic should not restrict themselves to the references here but should follow the citations in the given papers and use Science Citation

Index to check for more recent work.

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