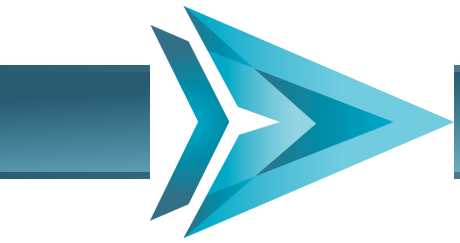

Surrogates: Emulating computer simulations

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1 Introduction

1.1 Purpose

This library will provide a suite of algorithms for emulating expensive computer simulations.

1.2 Scope

This library will replace the existing surrogate tools in Dakota and enrich these existing tools with additional state of the art surrogates and algorithms.

1.3 Overview

This library will consist of 5 main software components visible to the user at the highest level of abstraction:

- Function - A class, from which surrogates is derived whose interface represents the mathematical properties of a C_2 continous function, e.g supports evaluation of values, gradients and Hessians. evaluated
- Variables - A class defining the properties of the function variables, e.g. probability distribution, ranges, etc. We will support all current Dakota Variable types in addition to blocks of correlated variables whose distribution is known, data-based-variables whose distribution is computed from data, and compositions of all variables.
- Data - A class to store data returned by function and the associated samples of the function variables. This class will also contain fault information. We must provide modules that convert simple structures such as matrices and vectors of samples and values into this class.
- SurrogateFactory - A factory to construct a surrogate/approximation. Typical workflow will be generate a set of samples, evaluate function at those samples and build approximation. This call structure can be repeated iteratively to build up surrogates adaptively. We will also support the use and enrichment of archived data. This factor will support typical Dakota use-cases, however uses will be easily able to develop and add there own methods for building surrogates.

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- SurrogateAnalyzer - A factory for running various types of analysis on surrogate models, e.g. compute moments, sobol indices, etc. If certain surrogates support fast operations to compute these values, e.g. PCE can compute mean and variance analytically these specialized functions will be envoked, but other wise a default will be called.

Currently the above notions of function and surrogate builders and analysis are heaverly intertwined in Dakota. Our design will allow these distinct components to be separated. This will allow surrogates to become a standalone part of the dakota Model hierarchy and surrogate analyzers to become lightweight Dakota Iterators.

1.4 Requirements

The following is a list of requirements

- User flexibity. Design must support 'push-button' users that want hired wired behavior and power users that wish to develop their own surrogate methods or expose low-level functionality.
- Serialization of surrogates - Ability to save and load surrogate objects
- Python interface - be able to call both high-level and low-level functions using Python.
- Gaussian Process consolidation - Consolidate GP methods in Dakota. Extend GP to include estimation of hyper-parametersa and use PCE trend function.
- Surrogates for multiple QOI - Build a single surrogate for multiple QOI. Allow for composition of surrogate types.
- Exending variable class - Support all Dakota variable types as well as blocks of correlated variables whose distribution is known, data-based-variables whose distribution is computed from data, and compositions of all variables. Retirement of AleatoryDistParams in Dakota.
- Simple approximation classes. Separation of approximation and the code used to construct it. Particularly relevant in Pecos. RegressOrthogPolynomial contains PCE object but also regression methods used to build the PCE. Similarly for Sparse grids need to seperate approximation, either lagrange polynomials or PCE, from refinement tools For example, split current subspaces which are part of approximation from active subspaces being considered for refinement which should only been known to sparse grid builder
- Function Data. The function data class should have no notion of active and stored data we shold just use indexing to access the data needed.

2 Design

2.1 High-level interface

The following is an example of the typical workflow used to build a surrogate

Construct Surrogate Demonstration

```
// Configure options used to build surrogate
Teuchos::ParameterList factor_opts;
factory_opts.set(function, "target function");
factory_opts.set(data, "optional archived data");
factory_opts.set(PCE, "approximation type");
factory_opts.set("regression", "construction method");
//factory_opts.set("adapted-regression", "construction method");
factory_opts.set("OMP", "regression solver");
factory_opts.set("random", "sample type");
//factory_opts.set("optimal", "sample type");

// Build surrogate
Teuchos::RCP<Approximation> approx = SurrogateFactory(factory_opts);

// Analyze surrogate
Teuchos::ParameterList analyzer_opts;
analyzer_opts.set(MOMENTS, "analysis type");
Teuchos::RCP<AnalyzerMetrics> result = SurrogateAnalyzer(approx, analyzer_opts);

// Print metrics
std::cout << "Mean: " << result.get("mean") << std::endl;
std::cout << "Variance: " << result.get("variance") << std::endl;
```

2.2 Surrogate Interface

We will use a factory pattern to build a surrogate. The Surrogate factory will call lower level factories which are specific to each type of approximation. Approximation types can be added at these levels without the call to surrogate factory being modified. These new types can just be created by passing appropriate options via Teuchos::ParameterList.

Surrogate Factory

```
enum ApproxType {PCE,GP};
Teuchos::RCP<Approximation> surrogate_factory(const Teuchos::ParameterList opts){
  ApproxType approx_type = opts.get<ApproxType>("approximation type");
  switch (approx_type){
    case PCE : {
      return PCEFactory(opts, approx);
    }
    case GP : {
      return GPFactory(opts, approx);
    }
    default : {
      throw(std::runtime_error("Incorrect approximation type"));
    }
  }
}
```

2.3 Surrogate Analyzer

The surrogate analyzer will be implemented using a factory pattern. The analyzer will support various types of analysis on surrogate models, e.g. the computation of moments, sobol indices, etc. If certain

surrogates support fast operations to compute these values, e.g. PCE can compute mean and variance analytically these specialized functions will be envoked, but other wise a default will be called.

Surrogate Analyzer

```
enum AnalysisType {MOMENTS,SOBOL_INDICES};
Teuchos::RCP<AnaylzerMetrics> surrogate_anaylzer_factory(const Teuchos::ParameterList opts, Approxim
  AnalysisType analysis_type = opts.get<AnalysisType>("analysis_type");
  switch (analysis_type){
    case MOMENTS : {
      RealVector means, variances;
      Teuchos::ParameterList moment_opts;
      moment_opts.set(false, "compute_mean");
      moment_opts.set(false, "compute_variance");
      if (!approx.get("mean",means))
      // if specialized method does not exist use default
      moment_opts.set(true, "compute_mean");
      if (!approx.get("variance",variances))
      // if specialized method does not exist use default
      moment_opts.set(true, "compute_variance");
      compute_moments_using_sampling_carlo(
      approx,moment_opts,means,variances)
      break;
    }
    case SOBOL_INDICES : {
      RealMatrix sobol_indices;
      if (!approx.get("sobol_indices",sobol_indices))
      // if specialized method does not exist use default
      // opts can contain options like restricted indices
      compute_sobol_indices_using_sampling(approx,opts,sobol_indices);
      break;
    }
    default : {
      throw(std::runtime_error("Incorrect_approximation_type"));
    }
  }
}
```

2.4 Approximations

Approximations will all be derived from a base function class. The interface of the function class will be restricted to only those functions that represents the mathematical properties of a C_2 continous function, e.g supports evaluation of values, gradients and Hessians. Each approximation will only contain the methods relevant to its construction, e.g. PCE has build_basis_matrix and set_coefficients and GP has build_correlation_matrix and set_correlation_lenghts.

The basic approximation class hierarchy is depicted in Figure 1. This hierarchy will be extended as additional approximation types are added.

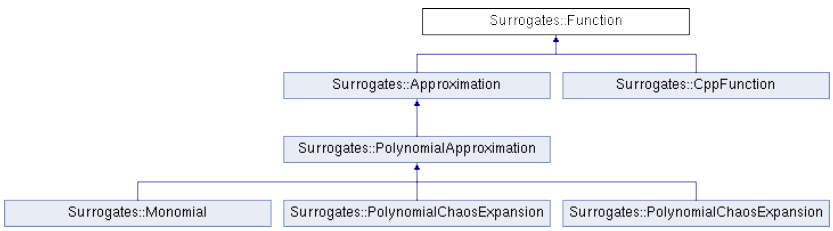


Figure 1: Function class hierarchy.

2.4.1 Function base class

Here we describe the abstract base class representation of a function $f(x)$ for a multivariate variable x. Functions derived from this class can either be C_0, C_1 or C_2 continuous. Regardlesd of the function regularity any derived class must implement value(), C_1 functions must implement gradient() and jacobian() and C_2 functions must implement hessian().

To avoid complexity of the function hierarchy we do not create seperate classes for C_0, C_1 and C_2 functions but rather only implement the functions necessitated by the function regularity. All other functions must raise an exception if called (these exceptions are implemented in this base class)

Public Member Functions

	Function () Default constructtor. More...
virtual	**~Function** () Destructor. More...
virtual void	**value** (const RealMatrix &samples, RealMatrix &values_out)=0 evaluate the vector-valued function $f(x)$ at a set of samples x. More...
virtual void	**gradient** (const RealMatrix &samples, int qoi, RealMatrix &gradients) evaluate the gradient of the ith QoI $\nabla f_i(x)$ of a vector valued function $f(x)$ at a set of samples x. More...
virtual void	**jacobian** (const RealVector &sample, RealMatrix &jacobian) evaluate the Jacobian $\nabla f(x)$ of a vector valued function $f(x)$ at a single samples x. More...
virtual void	**hessian** (const RealMatrix &samples, int qoi, RealMatrixList &hessians) evaluate the Hessian of the ith QoI $\Delta f_i(x)$ of a vector valued function $f(x)$ at a set of samples x. More...
virtual void	**set_options** (const Teuchos::ParameterList &opts) set options specific to the model More...
virtual void	**get_options** (Teuchos::ParameterList &opts) get the model specific options More...

Figure 2: Function base class member functions.

QUESTION: Do we have functions for value, gradient, hessian or do we have a function value(samples,opts) where opts specifies what of the three data to return.

2.5 Variables

Variables is a class defining the properties of the function variables, e.g. probability distribution, ranges, etc. There is almost no functionality in the base class except `num_vars`. The rest of the functionality is implemented in the derived class and variable transformations or approximations which use the derived class must know what additional functions are implemented. An example of a variable class is shown in Figure 3.

2.5.1 Variable Transformations

Surrogates will sometimes the users provided variables to be mapped to a set of variables that the approximation can use. E.g a PCE requires variables on canonical domains such as Uniform on $[-1, 1]$. These mappings are peformed by variable transformations. An example implementation for an affine transformation of bounded variables is shown below.

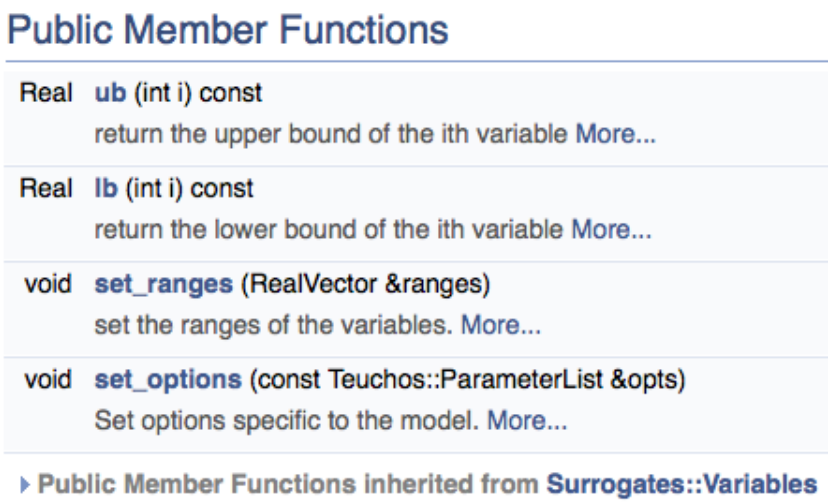


Figure 3: Example of a variables class.

Example of variable transformation code

```
void AffineVariableTransformation::
map_samples_from_user_space(const RealMatrix &samples,
RealMatrix &transformed_samples) const {
  int num_vars = boundedVars_->num_vars();
  if ( samples.numRows() != boundedVars_->num_vars() )
    throw( std::runtime_error("Samples have incorrect number of random variables") );

  int num_samples = samples.numCols();
  transformed_samples.shapeUninitialized(num_vars, num_samples);
  for ( int j=0; j<num_samples; j++ ){
    for ( int i=0; i<num_vars; i++ ){
      transformed_samples(j,i) =
        (samples(i,j)+1)/2.*(boundedVars_->ub(i)-boundedVars_->lb(i))+boundedVars_->lb(i);
    }
  }
}
```

Here is an example of using a variable transformation

3 Approximation Builders

The approximation factories call approximation builders. An example of how a builder may work is given below. This builder consists of two steps defining the approximation and the sampling the function and solving for its coefficients using regression. builders may call other builder in an inner loop. For example we may wish to iteratively add samples. In which case we would call this builder in an inner loop until an error estimate reaches a desired level of accuracy. In the example below we pass in a function but we could also pass in existing data.

Example of a surrogate builder

```
// Define the function variables
  RealVector ranges;
  define_homogeneous_ranges(num_vars, 0., 1., ranges);
  Teuchos::RCP<Variables> variables(new BoundedVariables());
  Teuchos::rcp_dynamic_cast<BoundedVariables>(variables)->set_ranges(ranges);

  // Define the variable transformation. Need to decide if a seperate
  // transformation should exist for approximation and for mapping samples
  // generated. For example approximation accepts samples in user x-space
  // but operates in a standardized u-space. But sample generator produces
  // samples in (possibly another standardized space) and must map these to
  // x-space, or even to approximation u-space.
  Teuchos::RCP<VariableTransformation> var_transform(new AffineVariableTransformation());
  var_transform->set_variables(variables);

// Initialize the approximation
  Teuchos::ParameterList monomial_opts;
  monomial_opts.set("max_total_degree",degree,
                    "max_degree_of_total-degree_polynomial_space");
  monomial_opts.set("num_qoi", num_qoi, "number_of_quantites_of_interest.");
  Monomial monomial;
  monomial.set_options(monomial_opts);
  monomial.set_variable_transformation(var_transform);
  IntMatrix basis_indices;
  compute_hyperbolic_indices(num_vars, degree, 1., basis_indices);
  monomial.set_basis_indices(basis_indices);

  // Generate the approximation coefficients using a regression based method
  Teuchos::ParameterList regression_opts;
  regression_opts.set("regression_type",SVD_LEAST_SQ_REGRESSION);
  regression_opts.set("num_samples",num_samples);
  regression_opts.set("sample_type","probabilistic_MC");
  RegressionBuilder builder;
  builder.set_target_function(model);
  builder.build(regression_opts, monomial);
```

QUESTION: DO we pass in target function and any data through ParameterList opts or through member functions?

3.1 Regression methods

For a given approximation type, there are a number of ways one might want to construt the approximation. For example we can use different types of regression to build a PCE, neural net etc, or we may want to build a pseudo spectral pce using different types of quadrature. In these cases we need factories to choose the builder sub-component, e.g. least squares or l1 minimization for regression based pce, or monte carlo or sparse grid quadrature for pseudo spectral pce. An example of such builders is given below.

Example builder for regression based approximations

```
// Generate samples to build approximation
int num_samples = opts.get<int>("num_samples");
std::string sample_type = opts.get<std::string>("sample_type");

// Create mc sampler and pass in sample type.
// For now hack support for uniform mc sampler
RealMatrix samples;
int seed = 1337;
Teuchos::RCP<VariableTransformation> var_transform =
  approx.get_variable_transformation();
generate_uniform_samples(approx.num_vars(), num_samples, seed,
                         *var_transform, samples);

// Evaluate the function at the build samples
RealMatrix values;
targetFunction_->value(samples, values);

//\todo consider having opts have multiple parameterLists
//each associated with a particular aspect of build
//e.g. opts = (sample_opts, regression_opts)
PolynomialApproximation& poly_approx =
  dynamic_cast<PolynomialApproximation&>(approx);

// Generate matrix of the linear system to be used in
// regression solve
RealMatrix basis_matrix;
poly_approx.generate_basis_matrix(samples,basis_matrix);

// Solve regression problem to get coefficients
Teuchos::RCP<LinearSystemSolver> solver =
  regression_solver_factory(opts);
RealMatrix coeffs, metrics;
solver->solve(basis_matrix, values, coeffs, metrics, opts);

// Set the approximation coefficients
poly_approx.set_coefficients(coeffs);
```

The solvers inheritance diagram is depicted in Figure 4. The hierarchy lets each class define specialized implementations of things like cross validation. Sparse solvers have a default implementation of iterative reweighting which they can call, the definition of this function DOES NOT exist in the base class. Specialization of sparse solver is shown in Figure 5

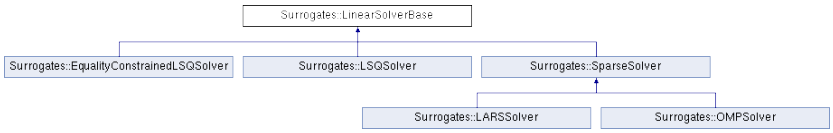
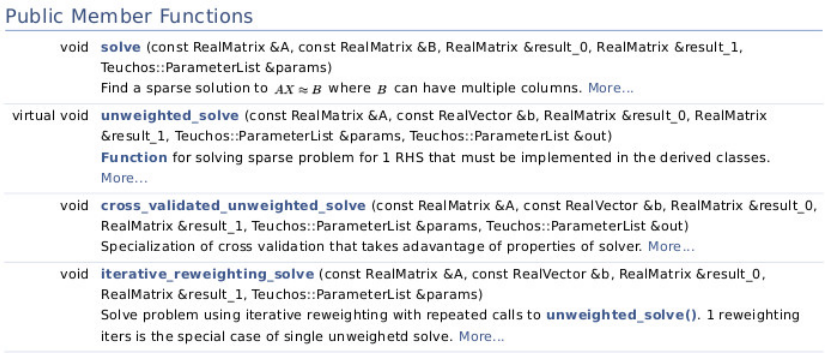


Figure 4: The regression solver hierarchy.

4 Integration with Dakota

Currently the notions of Approximation (DataFitSurrogate) and surrogate builders and analysis are heaverly intertwined in Dakota. Our design will allow these distinct components to be separated. This will allow Approximation to become a standalone part of the dakota Model hierarchy and surrogate analyzers to become lightweight Dakota Iterators.



Public Member Functions

void	**solve** (const RealMatrix &A, const RealMatrix &B, RealMatrix &result_0, RealMatrix &result_1, Teuchos::ParameterList &params) Find a sparse solution to $AX \approx B$ where B can have multiple columns. More...
virtual void	**unweighted_solve** (const RealMatrix &A, const RealVector &b, RealMatrix &result_0, RealMatrix &result_1, Teuchos::ParameterList &params, Teuchos::ParameterList &out) **Function** for solving sparse problem for 1 RHS that must be implemented in the derived classes. More...
void	**cross_validated_unweighted_solve** (const RealMatrix &A, const RealVector &b, RealMatrix &result_0, RealMatrix &result_1, Teuchos::ParameterList &params, Teuchos::ParameterList &out) Specialization of cross validation that takes adavantage of properties of solver. More...
void	**iterative_reweighting_solve** (const RealMatrix &A, const RealVector &b, RealMatrix &result_0, RealMatrix &result_1, Teuchos::ParameterList &params) Solve problem using iterative reweighting with repeated calls to **unweighted_solve()**. 1 reweighting iters is the special case of single unweighetd solve. More...

Figure 5: Sparse solver member functions. Only solve exists in baseclass

5 Variables

The Variables class is intended to encapsulate the creation, augmentation and realization of random variables. Single variables are characterized by such properties as probability distribution, ranges, hyperparameters, etc. A base class provides only the bare minimum via a `num_vars` attribute and a pure virtual `realize()` method. The rest of the functionality is implemented in the derived classes and require that variable transformations or approximations which use the derived classses to know what additional functions are implemented. (These could change.)

5.1 Requirements

The following are requirements the the Variables class must support in any design and implementation:

1. Functionality and use cases currently supported in the Pceos::RandomVariable class must be preserved.

2. Appropriate leveraging of Boost's stastical distributions should be preserved.

3. Consistent and performant extensions to available distributions should be added as needed, eg distributions based on underlying user-supplied data.

4. Extensions to multivariables ranging in type from iids to aggregations of varying distributions should be implemented in a way that preserves good performance while scaling up to high dimensions.

5. Correlations among variables should be able to be specified at construction or updated thereafter.

6. Transformations (including inverse when possible) should be supported with checks for appropriateness and consistency.

7. Where appropriate transformations should support distributions, e.g. return a new distribution, and realizations, e.g. map realizations from one underlying distribution to a value coreresponding to another distribution.

8. The previous transformation reuirements should apply to multivariables irespecting correlations where appropriate.

9. Variables (single and multiple) should be able to be serialzied for the purpose of export/import, e.g. for supporting restart capabilitiy

5.2 Creation APIs

The following examples illuatrate candidate APIs for creating single and multi-variable instances.

Example of single variable construction

```
Teuchos::ParameterList & var_opts;
var_opts.set("distribution", "Uniform");
var_opts.set("alpha", "-1.0");
var_opts.set("beta" , "1.0");
auto sVar = VariableFactory::create<>( var_opts );
```

Example of creating an independent IID multivariable

```
Teuchos::ParameterList & var_opts1;
var_opts1.set("distribution", "Uniform");
var_opts1.set("alpha", "-1.0");
var_opts1.set("beta" , "1.0");
auto sVar = VariableFactory::create<>( var_opts1 );

// Create a 10-dim uniform(-1.0, 1.0) iid multivariable
auto iidVar = VariableFactory::IID( sVar, 10 );
```

Example of creating an independent joint multivariable

```
Teuchos::ParameterList & var_opts1;
var_opts1.set("distribution", "Uniform");
var_opts1.set("alpha", "-1.0");
var_opts1.set("beta" , "1.0");
auto sVar1 = VariableFactory::create<>( var_opts1 );

Teuchos::ParameterList & var_opts2;
var_opts2.set("distribution", "Standard-Normal");
auto sVar2 = VariableFactory::create<>( var_opts2 );

auto mVar = VariableFactory::Joint( std::vector<VariableBase> {sVar1, sVar2} );
```

5.3 Sampling APIs

The following examples demonstrate how to obtain variates (realizations of random variables).

Example of variable realization (sampling)

```
auto sample = mVar.realize(); // would return a vector<Real> of size 2
                              // using the multivariable creation  example
```

5.4 Modification APIs

The following examples demonstrate how to reset existing instances of random variables and provide a possible means of efficient variate realizations for large dimension variables.

Resetting an existing uniform variable configuration

```
auto suVar = VariableFactory::create<>( var_opts );

std::cout << "Value 1 = " << suVar.realize() << std::endl;
auto old_config = suVar.param();
suVar.param(Surrogate::UniformDistribution<>::param_type {-1.0, 1.0});
std::cout << "Value 2 = " << suVar.realize() << std::endl;
suVar.param(old_range);
std::cout << "Value 3 = " << suVar.realize() << std::endl;
```