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Title: An Object-Oriented Optimization Systems

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AN OBJECT-ORIENTED OPTIMIZATION SYSTEMS

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ABSTRACT

We have described the implementation of a graphical programming tool in the object-oriented language, Smalltalk-80, that allows a user to construct a radiographic measurement model. The measurement model can be used to generate the measurements predicted by a given parameterized model of an experimental object. In this paper, we describe extensions to the graphical programming tool that allow it to be used to perform Bayesian inference on very large sets of object parameters, given real experimental data, by optimizing the likelihood or posterior probability of the parameters, given the real data.

1. INTRODUCTION

The object-oriented (OO) paradigm has recently attracted attention because of its promise for code reuse and ease of maintainence, in addition to the natural and intuitive language it promotes for discussion of software [3]. We have built and described an OO graphical programming tool [1] that allows a user to connect icons, which represent data transforms, on a canvas in order to define a data-flow diagram that acts on a user-defined object parameterization. In this paper, we describe an extension of the graphical programming tool that allows the user to interactively optimize a 1D functional of the output of the data-flow diagram with respect to object parameters. We discuss the advantages of programming the optimization tool in an OO language.

We believe that the optimization tool will be useful to scientists and engineers for orchestrating Bayesian inference and hypothesis testing of geometric object parameters given real radiographic data [2]. The general problem for which these tools are intended is the determination of an object of unknown shape and distribution, described by a user-defined parameterization, given limited data generated by a well-characterized, user-defined measurement system. The graphical programming tool, in conjunction with a likelihood function, allows the user to define a complete model of a measurement system. The maximum likelihood (ML) estimate of the parameters that describe the experimental object can be obtained using the optimization tool. Maximum *a posteriori* (MAP) estimates can also be obtained, if prior information is used.

2. THE OO PARADIGM

The OO paradigm is founded on the concept of an *object*. Objects have responsibilities, or *methods*, and data, or *attributes*. To talk about objects, either to one another in software analysis or design, or to the computer in a programming session, is natural and intuitive, since we think in terms of objects. Attributes are *encapsulated* by methods so that internal data storage, accessing, and manipulation, is not important to the "outside world", which can only obtain information about the attributes by *messaging* the object to perform some method. Encapsulation and messaging facilitate the construction of flexible, easy-to-understand software modules. *Classes* are templates of objects, and are contained in class hierarchies, wherein *subclasses inherit* methods and attributes from *superclasses*, so that code is re-used and sensibly organized. Finally, type-casting is eliminated with the use of *dynamic binding*.

We are using Smalltalk-80 and the VisualWorks programming environment from ParcPlace Systems in conjunction with C, Fortran, and X-Windows. Smalltalk-80 is a pure object-oriented programming language, which truly encourages object-oriented thinking. However, its poor performance in executing loops and numerical computations has forced us to use C and Fortran for numerically intensive computations and X-Windows for loop-intensive graphics.

3. AN OO GRAPHICAL PROGRAMMING TOOL

The graphical programming tool operates as follows (refer to Fig. 1). The user is presented with a canvas, on which appear buttons that allow the user to add items to, or delete items from, the canvas. The user can add or delete `Transforms` and `Connections`. `Transforms` map input `Data` to output `Data` and are represented on the screen by an icon. The user specifies

the data-flow by connecting one **Transform** to another using a **Connection**, which is represented on the screen as a set of connected line segments.

The **Transforms** are "living" objects, and the user can interact with them in several ways. He can see a description of a **Transform** and change the parameters that define it. The user can also message the **Transform** to display its output. This message is forwarded to the **Transform**'s **output** attribute, which is messaged to display itself. The fact that the **Transform** objects are alive distinguishes this graphical programming tool from one that allows a user to construct and visualize a script that contains a sequence of actions to be executed in a certain order.

We have written classes for several categories of **Transforms**, including **MultiInputSingleOutput** (**Add**, **Multiply**, **Subtract**), **SingleInputSingleOutput** (**Convolution**, **Exponential**, **Log**, **Log10**, **SqRt**, **Sin**, **Cos**, **LineIntegral**, **ParallelLineIntegral**) and no-input single-output (**Parameter** and its subclasses).

Parameter and its subclasses define the object model that is the input to the measurement model defined by the data-flow diagram. For example, a **GeometricObjectModel** has a **listOfComponents** that might contain a **Polygon2D**, a **Bezier2D**, a **Grid2D**, and a **UniformGrid2D**.

4. AN OO OPTIMIZER

Let the output of the measurement system model specified by the data-flow diagram be predicted data, $\hat{d}(\theta)$, where θ is a set of parameters that defines the object model. For example, $\theta = \{\theta_{ij}\}$ might be the set of density values in a **UniformGrid2D** of fixed size. If the user has data, d, that are generated by a real measurement system that corresponds well to the measurement system model, plus some additive noise, n, with probability distribution $P_N(n)$, then $P_N(d - \hat{d}(\theta))$ is a 1D functional on the output of the data-flow diagram, called the likelihood function. Optimizing $P_N(d-\hat{d}(\theta))$ over θ produces the ML estimate of θ given the data, d. If $P_\Theta(\theta)$ is a prior probability distribution over θ, then $\phi(\theta) = \log[P_N(d-\hat{d}(\theta))]+\log[P_\Theta(\theta)]$ is a 1D functional called the log posterior. Maximizing $\phi(\theta)$ over θ produces the MAP estimate of θ, given the data, d. Thus, the capability for optimizing 1D functionals of data-flow diagrams includes the capability for solving Bayesian inference problems.

We have extended the graphical programming tool to include Gaussian likelihood functions and the ability to optimize them with respect to object-model parameters using conjugate gradient (for unconstrained problems) and gradient descent (for constrained problems) methods.

4.1. The reverse adjoint method

We obtain the gradient of the log likelihood with respect to object model parameters ($\frac{\partial\phi}{\partial\theta_i}$) using a reverse adjoint technique, which implements the chain-rule for differentiation from back to front [4].

For example, let us define a simple measurement model (refer to Fig. 1) wherein $\hat{d}(x)$ denotes the data predicted by taking line integrals of a **UniformGrid2D** object model, x, using transform L, to produce path-lengths, y, which are then pointwise exponentiated to produce attenuations, z, and convolved with a point spread function represented by the matrix H to finally produce $\hat{d}(x)$. Then

$$\hat{d}(x) = H(E(L(x))) \tag{1}$$

is an approximation to a true radiographic measurement system that can be easily built using the graphical programming tool.

If our real data are d, and we assume that they are produced by adding white gaussian noise to the data predicted by the true object x_{TRUE}, then ϕ is just the norm of $\hat{d} - d$, and the derivative of ϕ w.r.t. $\hat{d}$ is just $d^* = 2(\hat{d} - d)$. The derivative of ϕ w.r.t. z is just $z^* = H^T d^*$, that is, the adjoint operator for the **Convolution** acting on the the **Data** passed back to it by the **Likelihood**. Similarly, the derivative of ϕ w.r.t. y is just $y^* = -\exp^{-y} \cdot z^* = E_y^T z^*$, where $\cdot$ is pointwise multiplication and y is the current input to the **Exponential**. Finally, the derivative of ϕ w.r.t. the object parameters x can be obtained by "backprojecting" the adjoint **Data** y^* to produce $x^* = L^T y^*$.

Thus, the derivative of ϕ w.r.t. x can be written:

$$\nabla\phi = L^T(E_y^T(H^T(2(\hat{d} - d)))) \tag{2}$$

This equation suggests a "reverse-adjoint" implementation. Each **Transform** must know how to calculate the derivative of its outputs w.r.t. its inputs. These are the "sensitivity matrices" L^T, E_y^T, H^T, which may well depend on the current input state of the **Transform**. Rather than calculating the sensitivity matrices explicitly and then having them operate on the adjoint **Data** set passed from the upstream **Transform**, we write adjoint operator codes that automatically process the adjoint **Data** set to produce a new adjoint **Data** set without calculating the sensitivity matrices explicitly. So, for example, we don't explicitly calculate E_y^T, which is diagonal but rather use the adjoint **Data** z^* to produce the adjoint **Data** $y^* = -\exp^{-y} \cdot z^* = E^T(y)z^*$, which only requires a vector multiply.

4.2. Extending the class hierarchy

Extending the responsibility of `Transforms` to include an associated adjoint gradient operation is easily accomodated in our OO programming environment. The adjoint method takes `Data` that has the structure of a `Transform` output and maps it into `Data` that has the structure of a `Transform` input. Dual to the data-flow mode of operation, where outputs of the data-flow diagram query previous `Transforms` to `generateOutput` until eventually `Parameters` are encountered and just return themselves, in the gradient-flow mode of operation `Parameters` query forward `Transforms` to `generateAdjointOutput` until eventually a `Likelihood` is encountered and returns the gradient of itself with respect to the present state of its `input`. Thus, the gradients flow backwards, or in reverse, until each `Parameter` eventually returns the gradient of the `Likelihood` with respect to itself.

`Connections` are also modified in order to propogate `Data` in both directions. When a `Connection` is told to `getData` it gets the `Data` from the previous `Transform` and sends it to the one upstream requesting it for `input`. When a `Connection` is told to `getAdjointData`, it gets the `adjointData` from the `Transform` upstream and sends it to the `Transform` downstream, requesting it as an `adjointInput`.

Note that, in general, computing the adjoint gradient operator requires that the `Transform` know the current state of its `input`, since the derivative may well depend on the `input` (the `Exponential`, e.g.). Thus, it is natural to bundle the `Transform` with its current state (stored in its `input`) as we have done.

`Parameters` are given extended responsibilities in order to accomodate the existing optimization strategies. In particular, all `Parameters` must be responsible for `add`'ing themselves to and `subtract`'ing themselves from any instance of the same Class. `Parameters` also must be able to `multiplyByScalar:aScalar`, find their `norm` and determine their `innerProductWith:anObject` for `anObject` that is an instance of the same class. Furthermore, we have made some `Parameters` capable of projecting themselves onto certain constraint sets, namely upper and lower bounds.

Since addition, subtraction, multiplication by scalar, norm, inner product, and constraint satisfaction are all the responsibility of `Parameters`, the `Optimizer` logic can be applied to very different types of optimizations problems, e.g. one or two-dimensional de-convolution, tomographic inversion, inversion from noisy nonlinear point functions, etc. The logic in the `Optimizer` can work for any vector space, regardless of its detailed structure. The detailed structure of the Parameters being optimized is taken care of in the implementation of the fundamental vector space operations (addition, multiplication by scalar, etc.). The encapsulation and polymorphism provided by the `Parameters` allows us to concentrate on building and adapting robust, abstract, optimization algorithms that can be widely employed.

4.3. Capabilities

The user specifies that a `Parameter` is to be optimized by connecting it to the `Optimizer`. The user can specify an optimization strategy (conjugate gradient or gradient descent), tolerances, and maximum number of iterations for the global search and each line minimization, and gets feedback on the current step size, number of global iterations, and the number of likelihood evalutions thus far.

At any point during the optimization, the user can interrupt the `Optimizer` so that he can see the present state of the solution (and `Data` predicted by the present solution) by using the graphical programming tool, which contains icons that represent the "live" `Data` being optimized. The present solution can be modified interactively using modelling tools that are called by interacting with the icon that represents the `Parameter` of interest. `Transforms` can also be changed at any time. The log likelihood and likelihood can be plotted as a function of step along the current gradient direction, and the effect of stepping along the gradient from the present solution for various step sizes can be visualized easily. These capabilities are very useful for understanding how the optimization is working, as well as for guiding the `Optimizer` toward a solution.

Note that a "global" derivative of ϕ w.r.t. object parameters is obtained by "local" message-passing and methods operating on encapsulated data. For example, one can change the fundamental representation of the object described above by having a `Polygon2D` parameterization θ that feeds into a `ConvertToUniformGrid2D` `Transform` to produce a `UniformGrid2D` x. One can use the previous graphical program as it is, and just insert the new `Transform` "before" x. Then x^*, the derivative of ϕ w.r.t. x, can be backpropogated to produce θ^*, the derivative of ϕ w.r.t. θ. The ability to cascade models of the experimental object suggests a "level of detail" approach to optimization (called multiscale if the successfully-refined parameterizations are `UniformGrid2Ds` with smaller pixels and called multigrid if the parameterizations are successfully-refined geometrical descriptions).

Finally, the `Optimizer` can be used to probe the confidence that the user should have in the final solution. The user can select two states of the `Parameter` set, say P_1 and P_2, and ask the Optimizer to provide a one-dimensional plot of the likelihood as a function of

the new **Parameter** set, $\alpha P_1 + (1-\alpha)P_2$. For example, one could perturb a **Polygon2D** solution, P_1, by moving a boundary vertex to a new location to produce P_2. Plotting the likelihood as a function of $\alpha P_1 + (1-\alpha)P_2$ would then reveal the confidence one should have in the position of that boundary vertex – a broad likelihood means that there are many positions of the boundary point that are equally likely, and so the position of that vertex should not be trusted.

5. SUMMARY

The advantages of an OO language are enormous in the context of graphical programming, graphical object modeling, and optimization. Not only did the OO paradigm make extending the graphical programming tool to include optimization easier than we expected, it also stimulated our creativity. The potential extensions we envision to interactive, graphical optimization using the foundation we have discussed in this paper are very exciting.

Our immediate future plans include extending the 2D radiographic measurement model to 3D polyhedra and volumetric grids. We also plan to incorporate other measurement models, such as range data (that measures exterior surface location) and surface velocity data. Ultimately, we envision 3D time-evolving object and measurement models that will be used to fuse data from a variety of experimental diagnostics.

6. REFERENCES

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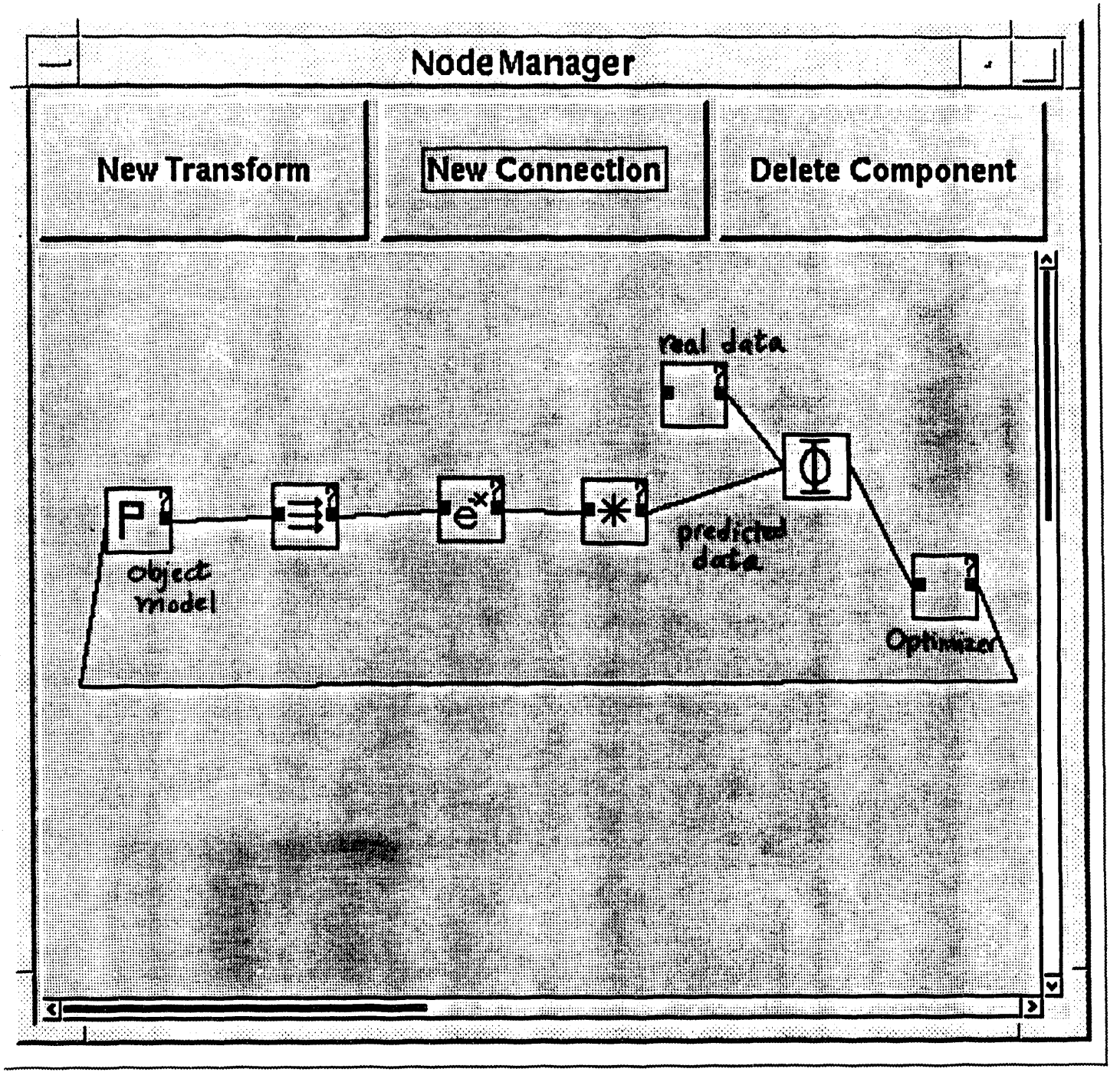


Figure 1a. The graphical programming tool canvas.

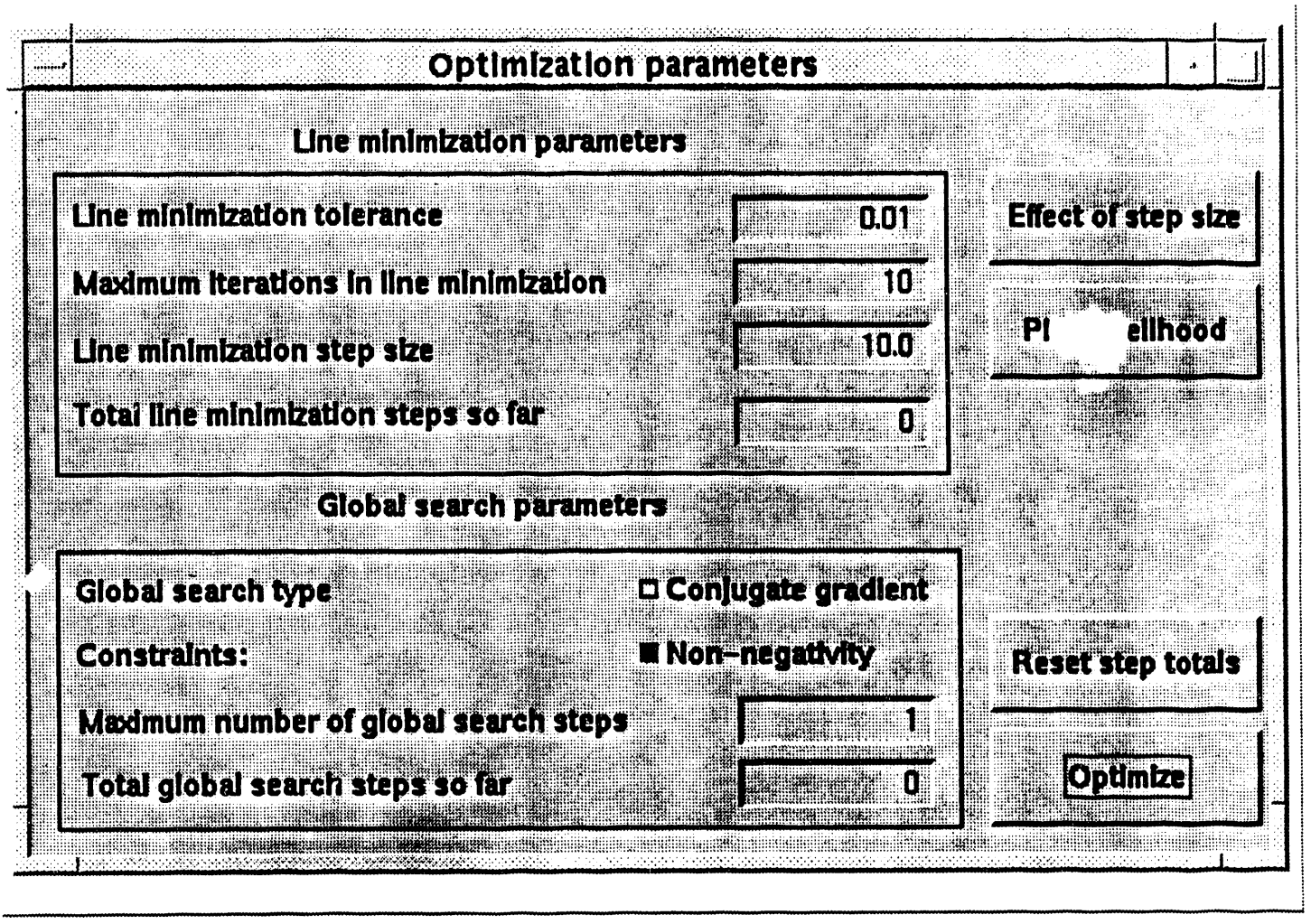
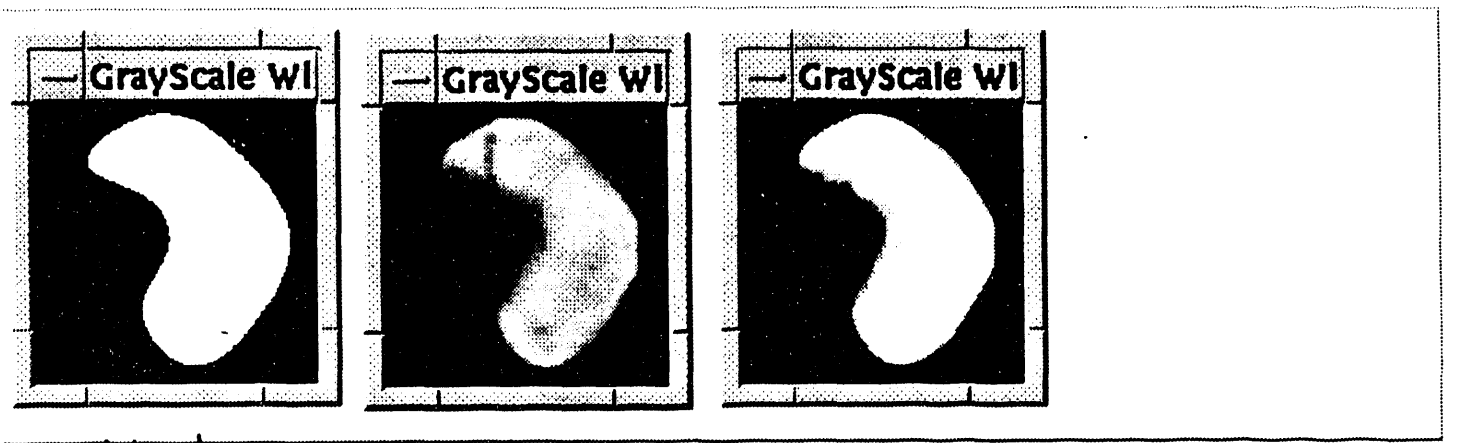


Figure 16. Optimizer interface



original

reconstruction with non-negativity constraint

reconstruction with non-negativity and upper bound constraints

Figure 1c. Reconstruction of 128×128 object using 6 views

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