VMl: A Functional Calculus for Scientific Discovery

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Outline of the Talk

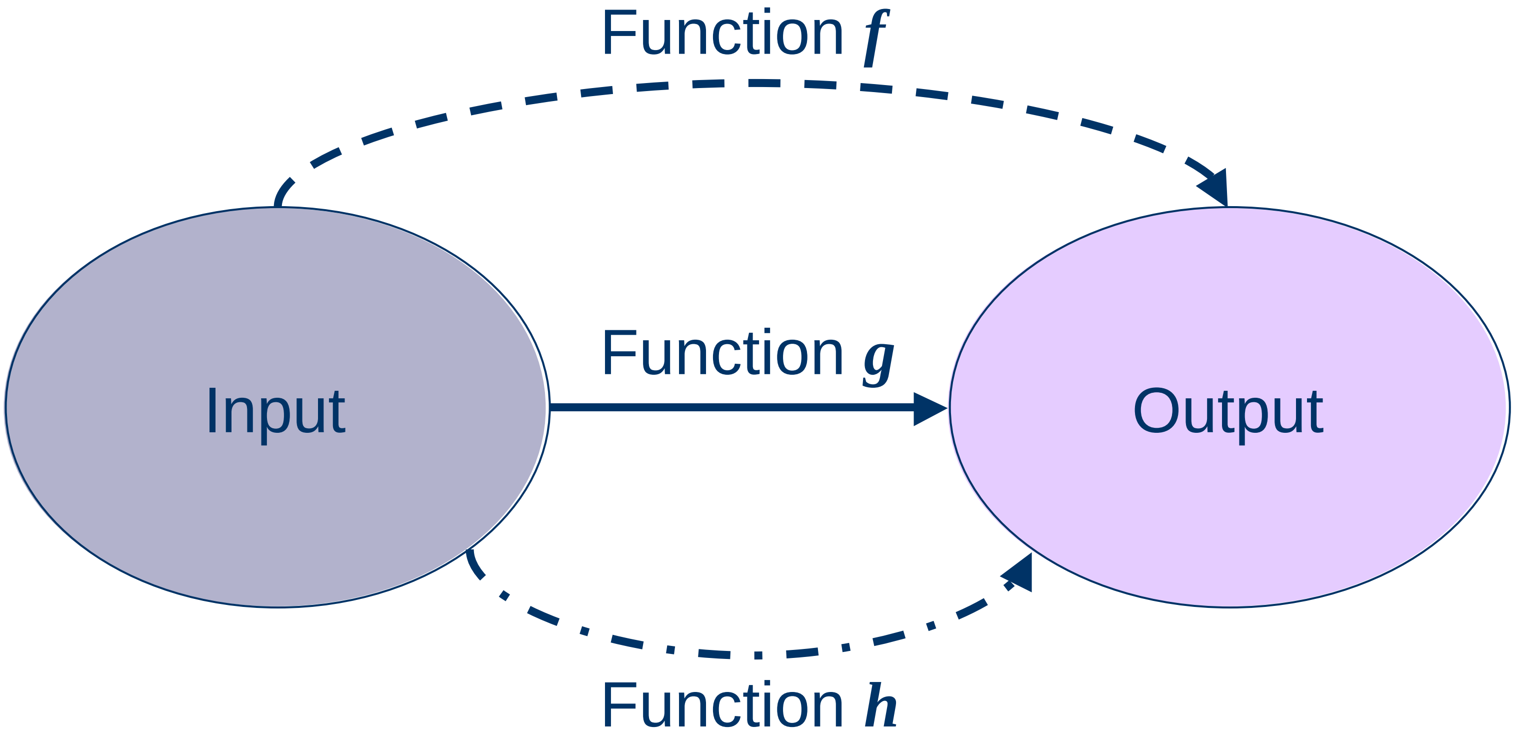
- Background
  - Discovery science and functional programming
- Simple VMλ
- VMλabl

Discovery Science [LNCS/LNAI 1532, 1721, 1967, 2226]

- A new area of computer science and artificial intelligence
- Originates in a project in Japan (http://www.i.kyushu-u.ac.jp/~arikawa/discovery/

- Aims to carry out a unified study of computer-aided *knowledge discovery*
- Based on formal logic, machine learning, data mining, etc.

Knowledge as Functions



Knowledge discovery = finding a "good" function

Knowledge Discovery by Functional Programming

- Fully automatic knowledge discovery is too difficult
  - $\Rightarrow$ Human interaction is essential
- What kind of interface is good for manipulating functions? (simple, expressive, fast, ...)
  - — Functional programming!

Example

- let data : (input $\times$ output) list =
  [(175.4, 73.9); (167.6, 66.1); (180.8, 81.2); ...]
  - List of pairs of two data (e.g., people's height and weight)
- let fitness :
  (input $\rightarrow$ output) $\rightarrow$ (input $\times$ output) list $\rightarrow$ float = ...
  - Tells how well a given function fits given data (according to some statistical criterion)
- let affine_approx :
  (input $\times$ output) list $\rightarrow$ (input $\rightarrow$ output) = ...
  - Creates the affine function $\boldsymbol{f(x) = ax + b}$ that fits given data best

How it works...

```
# let f = affine_approx data ;;
val f : input ® output = <fun>
# fitness data f ;;
- : float = 0.98
```

How it works…or does it?

```
# let f = affine_approx data ;;
val f : input ® output = <fun>
# fitness data f ;;
- : float = 0.98
```

Not really helpful – what *is* the function **`f`** ???

Naive Solutions

- Show the source code
  - Not very nice, because it can be too complex
- Pair the function with its representation

```
# let f' = affine_approx' data ;;
val f' :
  (float ® float) ´ repr =
  <fun>, AffineFun(1.03, -102.8)
```

  - Works, but too troublesome to do by hand
    - In particular because of a typing problem: functions with *different representations* may need to have the *same type*

Our Solution: "Views"

Pair of a value and its representation (of an extensible data type) that remembers "how the value was created"

([1] views for abstract types [Wadler 87])

```
# view AffineFun(a, b) = fun x ® a ´ x + b ;;
view AffineFun of float * float : float -> float
# let v = affine_approx' data ;;
- : (float -> float) view =
   <fun> as AffineFun(1.03, -102.8)
# vmatch v with AffineFun(a, b) ® (a, b) else ¼ ;;
- : float * float = (1.03, -102.8)
```

VML: ML Extended with Views

- Originally proposed in [Bannai et al. 2001]

◆ Defined in English prose only :-(

$$\Downarrow$$

■ Had problematic syntax and semantics :-(:-(

■ Never implemented successfully :-(:-(:-(

VMl: l-calculus extended with views

- Simple VMλ: every view must take just one argument
- VMλabl: views may take any number of arguments *in any order*
  - Implemented as an extension of OCaml/OLabl

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Syntax of Simple VMl

M (term) ::= ...		(standard λ-terms)
|	view V{x} = M_1 in M_2	(view definition)
|	V	(view constructor)
|	M_1\{M_2\}	(view application)
|	vmatch M_1 with V{x} $\Rightarrow$ M_2 else M_3	(view matching)
|	valof M	(view destruction)

Semantics of Simple VMl (1/2)

v (value) ::= ...		(standard λ-values)
|	⟨ε; V{x} = M⟩	(view constructor closure)
|	$V\{v_1\} = v_2$	(view)

$$\frac{V' \text{ fresh} \qquad \mathcal{E}, V \mapsto \langle \mathcal{E}; V'\{x\} = M_1 \rangle \vdash M_2 \Downarrow v}{\mathcal{E} \vdash \texttt{view}\ V\{x\} = M_1\ \texttt{in}\ M_2 \Downarrow v}\text{(E-VDe}$$

$$\frac{\mathcal{E} \vdash M_1 \Downarrow \langle \mathcal{E}'; V\{x\} = M' \rangle \qquad \mathcal{E} \vdash M_2 \Downarrow v \qquad \mathcal{E}', x \mapsto v \vdash M' \Downarrow v'}{\mathcal{E} \vdash M_1\{M_2\} \Downarrow V\{v\} = v'}\text{(E-VApp)}$$

Semantics of Simple VMl (2/2)

v (value) ::= ... (standard λ-values)

| ⟨ε; V{x} = M⟩ (view constructor closure)

| V{v$_1$} = v$_2$ (view)

$$\frac{\mathcal{E} \vdash M_1 \Downarrow V'\{v'\} = \_ \quad \mathcal{E}(V) = \langle \_; V'\{\_\} = \_\rangle \quad \mathcal{E}, x \mapsto v' \vdash M_2 \Downarrow v}{\vdash \texttt{vmatch}\ M_1\ \texttt{with}\ V\{x\} \Rightarrow M_2\ \texttt{else}\ M_3 \Downarrow v}\text{(E-VMatch-Suc}$$

$$\frac{\mathcal{E} \vdash M \Downarrow \_\{\_\} = v}{\mathcal{E} \vdash \texttt{valof}\ M \Downarrow v}\text{(E-ValOf)}$$

Type System of Simple VMl (1/2)

τ (type) ::= ...		(standard λ-types)
|	view{τ_1}τ_2	(view constructor type)
|	view{ }τ	(view type)

$$\frac{\Gamma, x : \tau \vdash M_1 : \tau_1 \qquad \Gamma, V : \mathtt{view}\{\tau\}\tau_1 \vdash M_2 : \tau_2}{\Gamma \vdash \mathtt{view}\ V\{x\} = M_1\ \mathtt{in}\ M_2 : \tau_2}\,(\text{T-VDe}$$

$$\frac{\Gamma \vdash M_1 : \mathtt{view}\{\tau\}\tau' \qquad \Gamma \vdash M_2 : \tau}{\Gamma \vdash M_1\{M_2\} : \mathtt{view}\{\}\tau'}\,(\text{T-VApp})$$

Type System of Simple VMl (2/2)

τ (type) ::= ...		(standard λ-types)
|	view{τ_1}τ_2	(view constructor type)
|	view{ }τ	(view type)

$$\frac{\Gamma(V) = \texttt{view}\{\tau\}\tau_1 \quad \Gamma \vdash M_1 : \texttt{view}\{\}\tau_1 \quad \Gamma, x : \tau \vdash M_2 : \tau_2 \quad \Gamma \vdash M_3 : \tau_2}{\vdash \texttt{vmatch}\ M_1\ \texttt{with}\ V\{x\} \Rightarrow M_2\ \texttt{else}\ M_3 : \tau_2}(\text{T-VMatc}$$

$$\frac{\Gamma \vdash M : \texttt{view}\{\}\tau}{\Gamma \vdash \texttt{valof}\ M : \tau}(\text{T-ValOf})$$

Type Soundness

If $\vdash M : \tau$,

then $\vdash M \not\Downarrow error$

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Partial Application of Multiple-Argument Views: The Problem

- *Partial application* of functions is a convenient feature of higher-order functional languages

...but does not extend to views *in a naive way*

Example (the originally proposed approach):

```
view V{x, y, z} = ... in
   let v' = fun x → fun z → V{x, 1 + 2, z} in
   vmatch v' with V{_, y', _} → ...
         (* forces unnatural evaluation of 1 + 2 *)
```

Our Solution: VMℓabl

Use *labeled arguments* [Garrigue & Ait-Kaci 94]

view V{ℓ_x = x; ℓ_y = y; ℓ_z = z} = ... in
    let v' = V{ℓ_y = 1 + 2} in
        (* natural to evaluate 1 + 2 here *)
    vmatch v' with V{ℓ_y = y'} $\rightarrow$ ...

Syntax of VM l abl

M (term) ::= ... (same as before)

| view $V\{\ell^+ = x^+\} = M_1$ in M_2 (view definition)

| $M_1\{\ell^+ = M_2{}^+\}$ (view application)

| vmatch M_1 with $V\{\ell^* = x^*\} \Rightarrow M_2$ else M_3 (view matching)

- X^* and X^+ are abbreviations for $X_1, \ldots, X_n$ where n ³ 0 or n > 0, respectively

Semantics of VMlabl (1/3)

v (value) ::= ... (same as before)

| ⟨ε; V{ℓ* = v*, m⁺ = x⁺} = M⟩ (view constructor closure)

| V{ℓ^+ = v_1^+} = v_2 (view)

$$\frac{V' \text{ fresh} \qquad \mathcal{E}, V \mapsto \langle \mathcal{E}; V'\{l^+ = x^+\} = M_1 \rangle \vdash M_2 \Downarrow v}{\mathcal{E} \vdash \texttt{view}\ V\{l^+ = x^+\} = M_1\ \texttt{in}\ M_2 \Downarrow v} \text{(E-VDe}$$

Semantics of VMlabl (2/3)

v (value) ::= ... (same as before)

| ⟨ε; V{ℓ* = v*, m$^+$ = x$^+$} = M⟩ (view constructor closure)

| V{ℓ^+ = $v_1{}^+$} = v_2 (view)

$$\frac{\mathcal{E} \vdash M_1 \Downarrow \langle \mathcal{E}'; V\{l_1^* = v_1^*, l_2^+ = x^+, l_3^+ = y^+\} = M\rangle \quad \mathcal{E} \vdash M_2^+ \Downarrow v_2^+}{\mathcal{E} \vdash M_1\{l_2^+ = M_2^+\} \Downarrow \langle \mathcal{E}', x^+ \mapsto v_2^+; V\{l_1^* = v_1^*, l_2^+ = v_2^+, l_3^+ = y^+\} = M\rangle} \text{(E-VApp-Par}$$

Semantics of VMlabl (3/3)

v (value) ::= ... (same as before)

| $\langle \varepsilon; V\{\ell^{*} = v^{*}, m^{+} = x^{+}\} = M\rangle$ (view constructor closure)

| $V\{\ell^{+} = v_1^{+}\} = v_2$ (view)

$$\frac{\begin{array}{c}\mathcal{E} \vdash M_1 \Downarrow \langle \mathcal{E}'; V\{l_1^* = v_1^*, l_2^+ = x^+\} = M\rangle \\ \mathcal{E} \vdash M_2^+ \Downarrow v_2^+ \quad \mathcal{E}', x^+ \mapsto v_2^+ \vdash M \Downarrow v\end{array}}{\vdash M_1\{l_2^+ = M_2^+\} \Downarrow V\{l_1^* = v_1^*, l_2^+ = v_2^+\} = v}\text{(E-VApp-Fu}$$

Type System of VMlabl

τ (type) ::= ... (same as before)

| view{ℓ* : τ*}τ (view / view constructor type)

$$\frac{\Gamma, x^{+} : \tau^{+} \vdash M_1 : \tau_1 \qquad \Gamma, V : \mathtt{view}\{l^{+} : \tau^{+}\}\tau_1 \vdash M_2 : \tau_2}{\Gamma \vdash \mathtt{view}\ V\{l^{+} = x^{+}\} = M_1\ \mathtt{in}\ M_2 : \tau_2}\text{(T-VDef}$$

$$\frac{\Gamma \vdash M_1 : \mathtt{view}\{l^{+} : \tau^{+}, l_0^{*} : \tau_0^{*}\}\tau \qquad \Gamma \vdash M_2^{+} : \tau^{+}}{\Gamma \vdash M_1\{l^{+} = M_2^{+}\} : \mathtt{view}\{l_0^{*} : \tau_0^{*}\}\tau}\text{(T-VApp)}$$

$$\frac{\begin{array}{c}\Gamma(V) = \mathtt{view}\{l^{*} : \tau^{*}, l_0^{*} : \tau_0^{*}\}\tau \qquad \Gamma \vdash M_1 : \mathtt{view}\{l_0^{*} : \tau_0^{*}\}\tau \\ \Gamma, x^{*} : \tau^{*} \vdash M_2 : \tau' \qquad \Gamma \vdash M_3 : \tau'\end{array}}{\Gamma \vdash \mathtt{vmatch}\ M_1\ \mathtt{with}\ V\{l^{*} = x^{*}\} \Rightarrow M_2\ \mathtt{else}\ M_3 : \tau'}\text{(T-VMatc}$$

Implementation of VMlabl

Translation by Camlp4 into OCaml/OLabl

- value of view constructor ⇒ function with labeled arguments
- representation of view ⇒ polymorphic variants
  - Recall "view = pair of a value and its representation (of an extensible data type)"

- Why polymorphic variants?
  (not abstract types, exceptions, etc.)
  - Allow pattern matching (unlike abstract types)
  - Don't require type declaration (unlike exceptions)

Conclusions

- We have formalized and implemented VML (ML with views), a functional programming language for scientific knowledge discovery
- Real applications are explained in a previous paper [Bannai et al. 2001]
  - Detection of gene regulatory sites
  - Characterization of N-terminal protein sorting signals

◆ People *do* find functional programming (and its theories) useful, if they open their mind