

From Data to Knowledge

Michael C. Ferris
(joint work with Olvi Mangasarian, Edward Wild)

University of Wisconsin, Madison
NSF Grants IIS-0511905, DMI-0521953 & DMS-0427689

November 3, 2007

Knowledge is Summary of Data

Points, records, images		data
Zip file	compression \iff	knowledge
Visualization	summary \iff	knowledge
Progressive meshes/JPEG	inference \iff	knowledge
Animations (foreground vs background)	level of detail \iff	knowledge
Robot football (field, location of players)	state \iff	data
Where to pass	implications, action \iff	knowledge

Knowledge is often formulated as an implication

Medical Applications

Symptoms given to doctor [partial information]

What is ailment?	determine state	\iff	knowledge
What is treatment?	action	\iff	knowledge
What is prognosis?	prediction	\iff	knowledge

Medical Applications

Symptoms given to doctor [partial information]

What is ailment? determine state \iff knowledge

What is treatment? action \iff knowledge

What is prognosis? prediction \iff knowledge

- Clinical images (of different biological response) [data conflict]
- Uncertainty of tumor and organ location [data uncertainty]
- Required treatment plan: adaptive (feedback) \iff knowledge

Medical Applications

Symptoms given to doctor [partial information]

What is ailment? determine state \iff knowledge

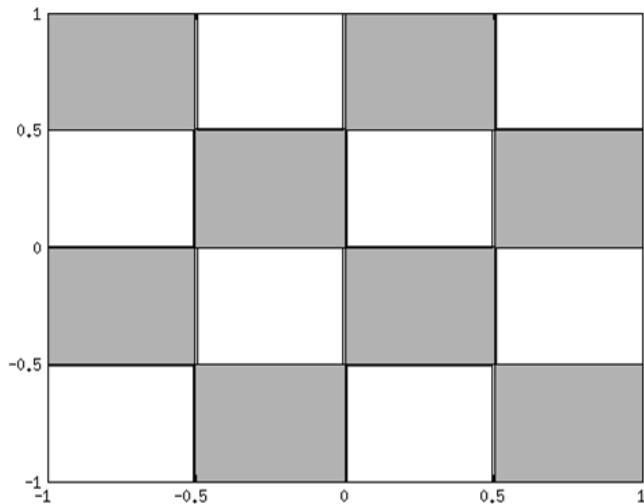
What is treatment? action \iff knowledge

What is prognosis? prediction \iff knowledge

- Clinical images (of different biological response) [data conflict]
- Uncertainty of tumor and organ location [data uncertainty]
- Required treatment plan: adaptive (feedback) \iff knowledge

ITR funding facilitated domain expert interaction

Checkerboard Dataset Black and White Points in \mathbb{R}^2



Multiple representations of knowledge

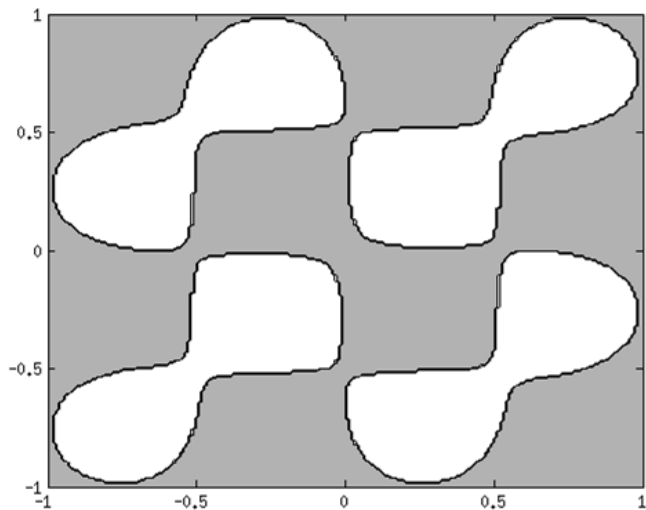
- 1 Bitmap image
- 2 Patches plus anchor points
- 3 Compression using replication
- 4 Nonlinear function “classifier” $f(x) = \sum_i K_i(x)u_i$

Basis pursuit, “sparse” L_1 (signal processing) models, reduced SVM

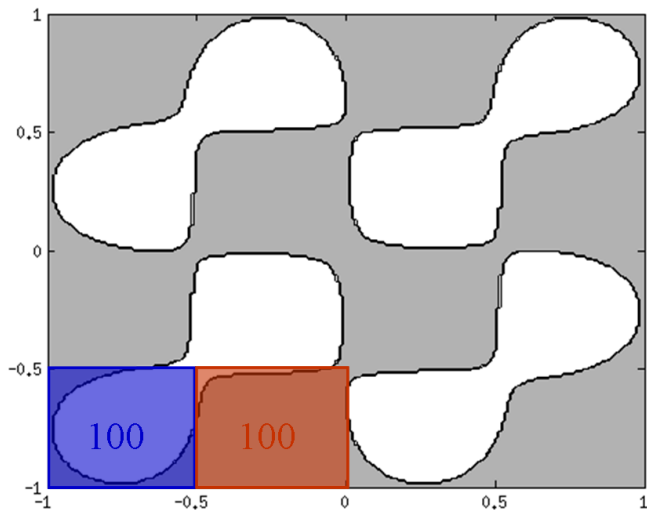
- Useful in different contexts
- Possibly problem domain specific
- Varying degrees of complexity

Models encode representations; Optimization is key to recovery

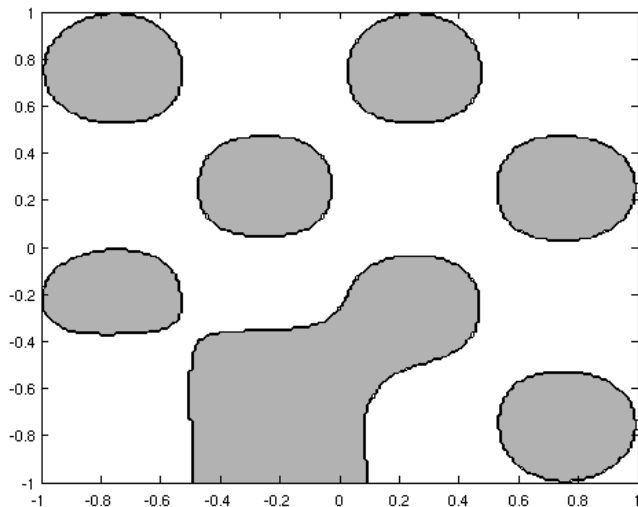
Checkerboard Classifier Using 16 Center Points



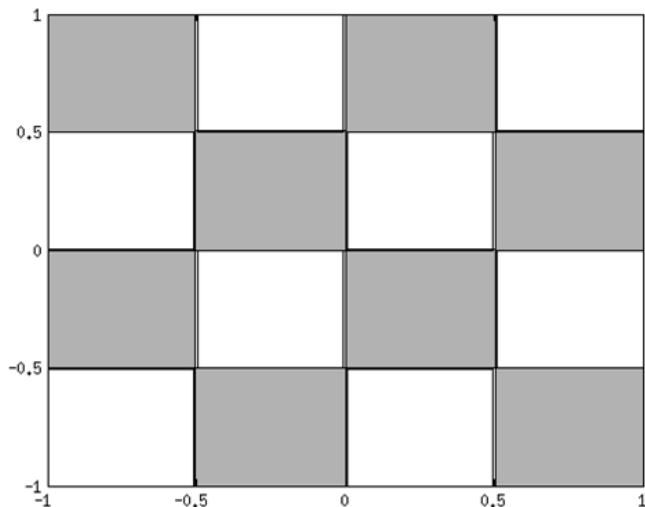
Prior Knowledge for 16-Point Checkerboard Classifier



Checkerboard Classifier with Knowledge as Extra Data



Checkerboard Classifier With Knowledge and 16 Points



Overview

Rigorous theory, good models, powerful computation

Use of knowledge

- Theoretical underpinnings
- Natural incorporation of knowledge
- Examples of application

Models based on “robust” and “generalized constraints”

- Use of powerful modeling tools coupled with cyber-infrastructure
- Training, and tuning via grid
- Large distributed datasets

Incorporating Knowledge

- Utilizing only given data may result in a poor classifier or approximation
 - ▶ Points may be noisy
 - ▶ Sampling may be costly
 - ▶ Overfitting/imbalanced data
- Use “summarization” of prior knowledge to improve the classifier or approximation
- Require “natural” imposition of knowledge understandable to humans

Rigorous Theory

Theorem (of the alternative, nonlinear)

Under appropriate assumptions, exactly one of the following two systems has a solution:

$$(I) : \quad \exists x \in \Gamma : g(x) \leq 0, f(x) < \gamma(x)$$

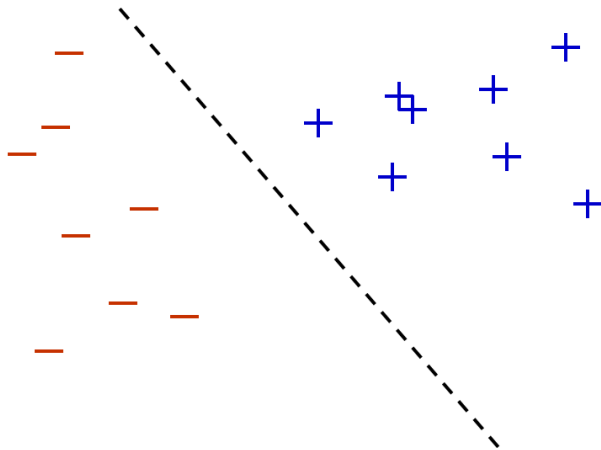
$$(II) : \quad \exists v \geq 0 : v^T g(x) + f(x) - \gamma(x) \geq 0, \quad \forall x \in \Gamma$$

Thus, if (II) has solution then:

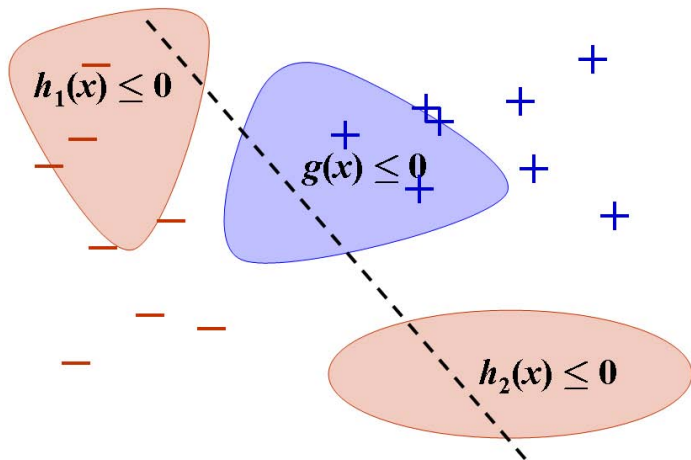
$$g(x) \leq 0 \implies f(x) \geq \gamma(x), \quad \forall x \in \Gamma$$

(Previous work involved “kernelizing” knowledge - effective but not transparent).

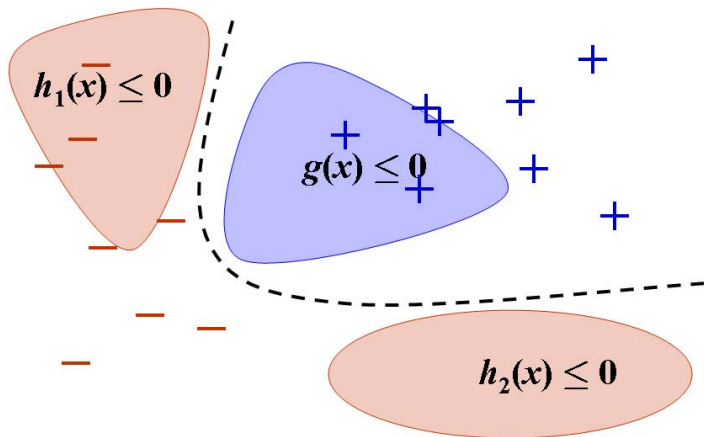
Knowledge Incorporation Example



Knowledge Incorporation Example



Knowledge Incorporation Example



Model Incorporating Knowledge

Linear semi-infinite program

$$\begin{aligned} \min_{(u,s,y \in Y, v \geq 0)} \quad & \|u\|_1 + v \|s\|_1 \\ \text{s.t.} \quad & -s_j \leq f(A_j \cdot) - y_j \leq s_j, \quad \forall j \\ & v^T g(x) + f(x) - \gamma(x) \geq 0, \quad \forall x \in \Gamma. \end{aligned}$$

Model Incorporating Knowledge

Linear semi-infinite program

$$\begin{aligned} \min_{(u,s,y \in Y, v \geq 0)} \quad & \|u\|_1 + v \|s\|_1 \\ \text{s.t.} \quad & -s_j \leq f(A_j \cdot) - y_j \leq s_j, \quad \forall j \\ & v^T g(x) + f(x) - \gamma(x) \geq 0, \quad \forall x \in \Gamma. \end{aligned}$$

Discretize (to get LP) and add trade-off parameter

$$\begin{aligned} \min_{(u,s,y \in Y, v \geq 0, z \geq 0)} \quad & \|u\|_1 + v \|s\|_1 + \sigma \|z\|_1 \\ \text{s.t.} \quad & -s_j \leq f(A_j \cdot) - y_j \leq s_j, \quad \forall j \\ & v^T g(x^i) + f(x^i) - \gamma(x^i) + z_i \geq 0, \quad \forall i. \end{aligned}$$

Global versus local

- Local \equiv “training data”
- Global \equiv “generalization”

Classification-Based Global Optimization

- Build a “classifier” to predict level sets of objective based on data
- Classifier is “cheap” to evaluate
- Use classifier to target evaluations in regions that are promising
- Component of WISOPT software
- Application to simulation calibration, e.g. Wisconsin Breast Cancer Epidemiology

Powerful Computation

- Global models incorporating (domain) knowledge (reflect more accurately our underlying knowledge of the system)
- Use of grid computation (eg. GAMS/grid, Condor, Sun Grid engine) to enhance global search
- Build a tractable “non-convex” model

$$\min_{i=1,\dots,N} Q_i(x)$$

to approximate a non-convex objective

- Use high performance computing to evaluate model minimizers in parallel
- Application to protein docking

Predicting Breast Cancer Recurrence Within 24 Months

Wisconsin Prognostic Breast Cancer (WPBC) dataset

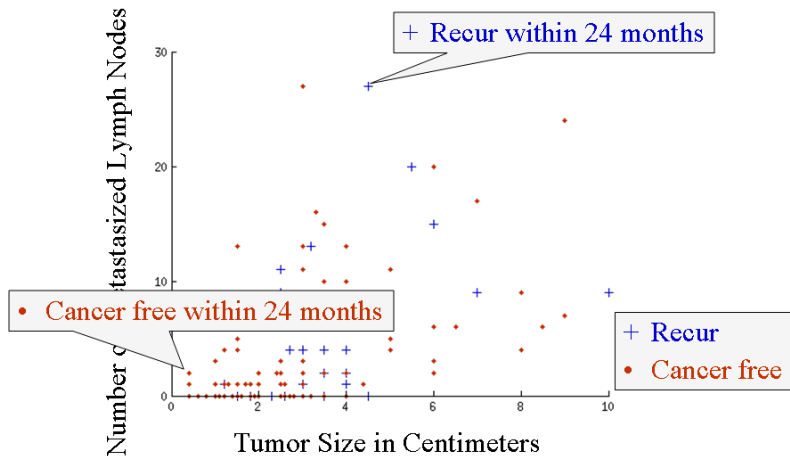
- 155 patients monitored for recurrence within 24 months
- 30 cytological features
- 2 histological features: number of metastasized lymph nodes and tumor size

Predicting Breast Cancer Recurrence Within 24 Months

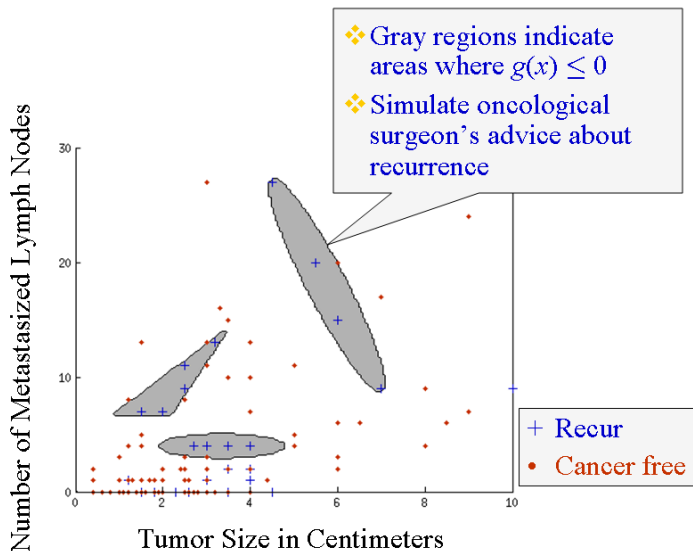
Wisconsin Prognostic Breast Cancer (WPBC) dataset

- 155 patients monitored for recurrence within 24 months
 - 30 cytological features
 - 2 histological features: number of metastasized lymph nodes and tumor size
-
- Predict whether or not a patient remains cancer free after 24 months
 - 82% of patients remain disease free
 - **86% accuracy** (Bennett, 1992) best previously attained
 - Prior knowledge allows us to incorporate additional information to improve accuracy

Generating WPBC Prior Knowledge



Generating WPBC Prior Knowledge



WPBC Results

Classifier	Misclassification Rate
Without Knowledge	18.1%
With Knowledge	9.0%

49.7% improvement due to knowledge

35.7% improvement over best previous predictor

Conclusion

Utilize nonlinear prior knowledge in classification/approximation

- Implemented as linear inequalities in a linear programming problem
- Knowledge appears transparently

Demonstrated effectiveness

- Real world problem from breast cancer prognosis

Future work

- Prior knowledge with more general implications
- Generate prior knowledge for real-world datasets
- See www.cs.wisc.edu/~olvi/nsf04

Possible Funding Opportunities

- Privacy notions: infer a summary without identifying subjects
 - ▶ mental health
 - ▶ finance
 - ▶ health-care (features and individuals)
- Interdisciplinary (knowledge) incorporation
 - ▶ biological, imaging, ultrasound, transaction
- Imprecise, inaccurate, uncertain data
- Novel modeling paradigms
- Cyber-infrastructure resources applied in application domains