Autologistic Regression Models, With Application to Segmentation of Hyperspectral Satellite Imagery

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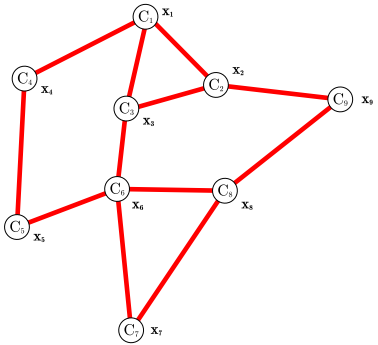
Outline

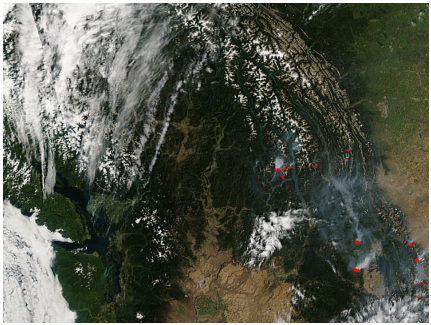
The technical content:



Autologistic regression for binary variables $\mathbf{C}$, with complex association, and covariate information $\mathbf{X}$.

- There are a few model variants.
- Claim: *it matters* which one you choose.

The application:



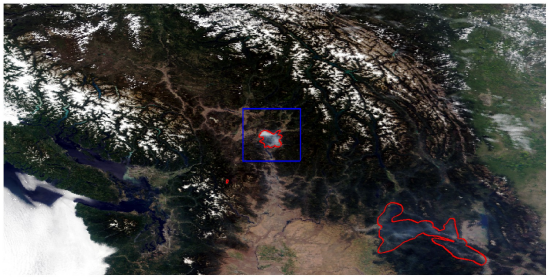
Where is the smoke in this picture?

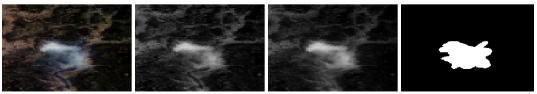
Motivating application

Remote sensing for smoke monitoring

Earth-orbiting satellites help study large-scale environmental phenomena.

Our interest: smoke from forest fires.





Original image | Green | Blue | True class

Data: MODIS images

- 1 per day, 143 days
- 1.2 Mp each
- Centered at Kelowna, BC
- Hand-drawn smoke areas

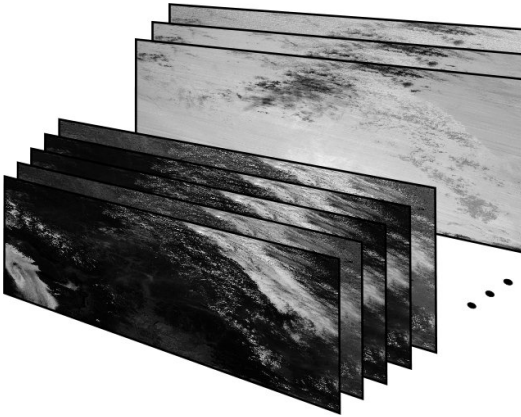
Goal: classify pixels into *smoke*/*nonsmoke*

Why?

- Health studies
- Model input or validation
- Monitoring & archiving

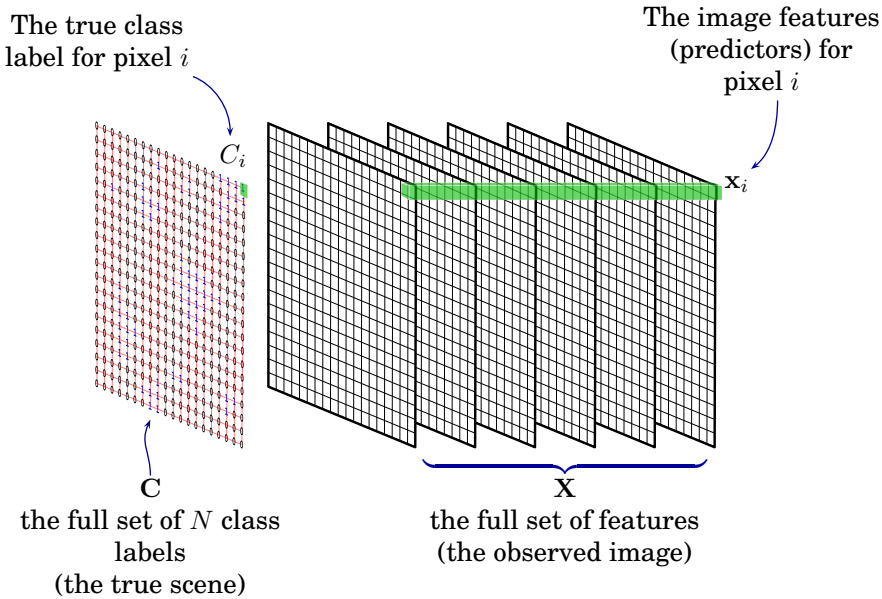
Data characteristics

- *Binary responses* (smoke/nonsmoke).
- Spectra at each pixel are *covariates* for predicting smoke.
- *Hyperspectral* images: a *high-dimensional* predictor space.
- Expect *spatial association*.



35 image planes
+
higher order terms

Notation


The true class label for pixel i
The image features (predictors) for pixel i
C_i
$\mathbf{x}_i$
$\mathbf{C}$
the full set of N class labels
(the true scene)
$\mathbf{X}$
the full set of features
(the observed image)

Autologistic regression models

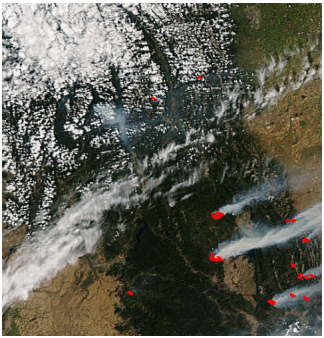
Spatial Associations

Image segmentation = pixel classification.

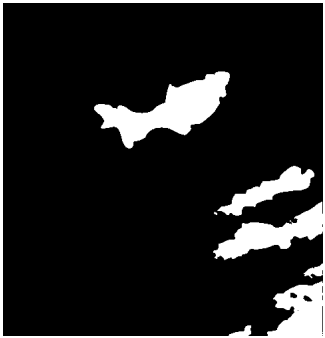
If independent pixels ⇒ Use standard classification technology.

But smoke/nonsmoke regions are *spatially smooth*.

RGB working image



The true scene



Model-Based Approaches

Many *ad hoc* ways to let pixels influence each other.

Model-based approach: *Markov random fields (MRFs)*.

- graphical model
- popular in computer vision

Image model (how to do?)

MRF model for the true scene

Generative model: $p(\mathbf{C}|\mathbf{X},\theta) \propto p(\mathbf{X}|\mathbf{C},\theta)p(\mathbf{C},\theta)$

Discriminative model: $p(\mathbf{C}|\mathbf{X},\theta) = \eta(\mathbf{X},\theta)$ $\Leftarrow$ *regression*

"conditional random field"

We will use the discriminative approach.

Model $p(\mathbf{C}|\mathbf{X},\theta)$ directly as a MRF.

Hammersley–Clifford theorem

Joint PMF can be expressed as a product of *potential functions*, one for each *maximal clique*.

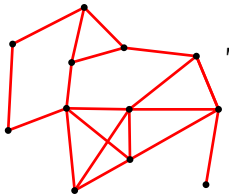
$\mathcal{M}$ = the set of maximal cliques.
$\mathbf{C}_m$ = the variables in the m^{th} clique. Then

$$p(\mathbf{c}) = \frac{1}{Z} \prod_{m \in \mathcal{M}} \phi_m(\mathbf{c}_m)$$

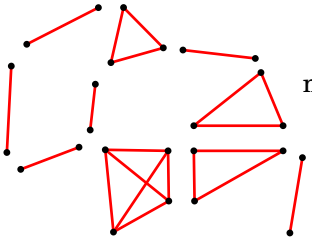
Customary to write the joint density as *Gibbs distribution* form,

$$p(\mathbf{c}) \propto e^{Q(\mathbf{c})}$$

where $Q(\cdot)$ is the *negpotential function*.



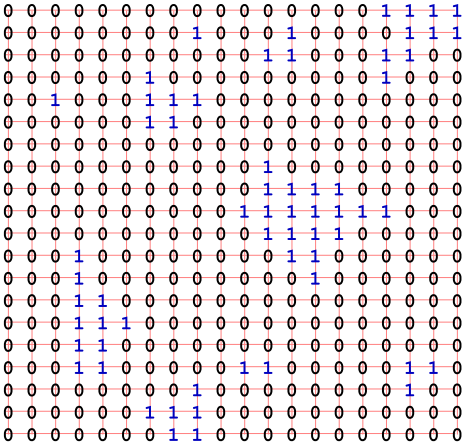
The MRF



Its maximal cliques

The Autologistic Model

- A Markov random field of **binary random variables**.
- For now, use zero/one coding: $\mathbf{C}_i \in \{0, 1\}$.
- The graph is a **regular, square grid**.
- Nothing new
  Physics: Ising model
  Statistics: Besag (1974)



The Autologistic Model (2)

Joint PMF:

$$\Pr(\mathbf{C} = \mathbf{c}|\boldsymbol{\alpha}, \boldsymbol{\lambda}) = \frac{1}{Z(\boldsymbol{\alpha}, \boldsymbol{\lambda})} \exp\left(\underbrace{\sum_{i \in \mathcal{V}} \alpha_i c_i}_{\textbf{unary terms}} + \underbrace{\sum_{(i,j) \in \mathcal{E}} \lambda_{ij} c_i c_j}_{\textbf{pairwise terms}} \right)$$

unary terms (one per vertex)

pairwise terms (one per edge)

- Positive α_i values favor $+1$ class.
- Setting $\lambda_{ij} > 0$ favors *locally smooth* configurations ($C_i = C_j$).
- Typically set $\lambda_{ij} = \lambda, \forall i, j$

Conditional distributions:

Let $\pi_i = \Pr(C_i = 1|\text{all other } C)$. Then can show:

$$\log\left(\frac{\pi_i}{1 - \pi_i}\right) = \alpha_i + \sum_{j \sim i} \lambda_{ij} c_j$$

j is a neighbour of i

Autologistic *Regression*

Put covariates in the unary part: $\alpha_i = \mathbf{x}_i^T \boldsymbol{\beta}$.

Pairwise coefficients: $\lambda_{ij} = \lambda$.

Then:

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = \mathbf{x}_i^T \boldsymbol{\beta} + \lambda \sum_{j \sim i} c_j.$$

Interpretation:

- Unary part is a linear predictor.
- $\mathbf{x}_i^T \boldsymbol{\beta}$ determines conditional log-odds of $C_i = +1$ in the absence of spatial effects.
- Pairwise λ determines strength of neighbour effects.
- *Setting $\lambda = 0$ reverts to standard logistic regression*.

A centered version

Caragea & Kaiser (2009)
"Autologistic models with interpretable parameters"
Hughes, Haran, & Caragea (2011)
"Autologistic models for binary data on a lattice"

- The neighbour sum $\sum c_j$ increases log-odds unless all neighbours are zero.
  $\Longrightarrow$ Estimates of $\boldsymbol{\beta}, \lambda$ are strongly coupled

- Strongly recommended a *centered autologistic model*:

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = \mathbf{x}_i^T\boldsymbol{\beta} + \lambda\sum_{j\sim i}(c_j - \mu_j)$$

  where $\mu_j = \mathrm{E}[Y_j|\lambda = 0]$ is the independence expectation.

Estimation Issues

Estimation is made hard by the normalizing constant.

Existing possibilities

1. Ignore spatial association (logistic regression, large n, large p).
2. Pseudolikelihood (PL): $L(\boldsymbol{\beta}, \lambda) \approx \prod_{\text{img}} \prod_{i=1}^{n} \text{logit}(\pi_i)$
3. Monte Carlo ML
4. Bayesian approach

} *Hughes et al. use perfect sampling; recommend PL for large n.*

Problems

- We have $\sim 10^8$ pixels
- We have thousands of predictors, need model selection
- We're still developing models—rapid evaluation of candidates is beneficial

Some claims about coding and centering

Model variants

- Binary variables do not have to take values 0 and 1.
- In general, let them have coding $\{\ell, h\}$
- We're most interested in
  $\{0, 1\}$, used in statistics and sometimes in computer vision
  $\{-1, 1\}$, used in physics and sometimes in computer vision
- And we have two possibilities:
  centered, or
  standard (not centered)

Are all these model variants just parameter transformations, or are they distinct models?

If not the same, what are the differences?

In the following , say $f_1(\mathbf{z}; \boldsymbol{\theta}_1)$ and $f_2(\mathbf{y}; \boldsymbol{\theta}_2)$ are *equivalent* if for any $\boldsymbol{\theta}_2$ there exists a $\boldsymbol{\theta}_1^*$ such that the two models assign the same probability whenever $\mathbf{z}$ and $\mathbf{y}$ represent the same configuration.

A general form of the model

If we let the coding be $\{\ell, h\}$ and define the centering adjustment

$$\boldsymbol{\mu}_{\boldsymbol{\alpha}} = \begin{cases} \mathbf{0} & \text{for a standard model} \\ [\mu_1^{\alpha} \cdots \mu_n^{\alpha}]^T \text{ with } \mu_i^{\alpha} = \dfrac{\ell e^{\ell\alpha_i} + h e^{h\alpha_i}}{e^{\ell\alpha_i} + e^{h\alpha_i}} & \text{for a centered model} \end{cases}$$

Then the *autologistic (AL)* PMF is

$$f_{\mathbf{C}}(\mathbf{c}; \boldsymbol{\alpha}, \lambda) \propto \exp(\mathbf{c}^T\boldsymbol{\alpha} - \lambda \mathbf{c}^T \mathbf{A}\boldsymbol{\mu}_{\boldsymbol{\alpha}} + \frac{\lambda}{2}\mathbf{c}^T\mathbf{A}\mathbf{c}),$$

where $\mathbf{A}$ is the adjacency matrix.

And the logit form is

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = (h-\ell)\left(\alpha_i + \lambda \sum_{j\sim i}(c_j - \mu_j^{\alpha})\right)$$

To obtain the *autologistic regression (ALR)* model, just plug in $\boldsymbol{\alpha} = \mathbf{X}\boldsymbol{\beta}$

Autologistic models are equivalent

Theorem 1

All AL models are equivalent, irrespective of coding or centering.

Sketch of proof:

- If $\mathbf{z}$ and $\mathbf{y}$ have different coding, they are related by

$$\mathbf{z} = a\mathbf{y} + b\mathbf{1}$$

  whenever they represent the same configuration.
- Use this to equate PMFs of $\mathbf{z}$ and $\mathbf{y}$
- Obtain an explicit parameter transformation from one model to the other

Autologistic regression models are NOT equivalent

Theorem 2

Different ALR models are not, in general, equivalent.

Sketch of proof:

- Follow logic of Theorem 1.
- Transformation between model only exists if an overdetermined system (n equations, p unknowns) can be solved for $\boldsymbol{\beta}$.
- Coefficients of the system depend on arbitrary $\mathbf{X}$.
- System is linear for standard models, nonlinear for centered ones.

This means

- standard, zero/one
- standard, plus/minus
- centered, zero/one
- centered, plus/minus

Are *four different probabilistic structures*.

Advantages of standard, plus/minus model

Claim: the standard model with $\{-1, 1\}$ coding is the best choice.

Why?

1. It resolves the asymmetry of the standard model without the awkward $\boldsymbol{\mu_\alpha}$ term:

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = 2\left(\mathbf{x}_i^T\boldsymbol{\beta} + \lambda\sum_{j\sim i} c_j\right)$$

   Sign of pairwise term depends on majority vote.

2. It "decouples" $\boldsymbol{\beta}$ and λ better than centering (evidence to follow).

2. It allows a convenient *plug-in estimation* of λ ...

An estimation shortcut for λ

Proposal: plug-in estimation

a) Use independence (logistic) to get $\hat{\boldsymbol{\beta}}$
   - Including model selection
   - Sample pixels if neccesary to reduce n to manageable size

b) Choose $\hat{\lambda}$ to optimize predictive power

Rationale

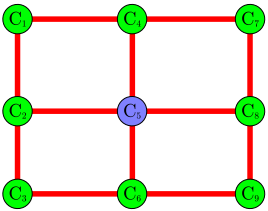
Treat λ as a smoothing parameter.

- Assuming independence, $\hat{\boldsymbol{\beta}}$ captures how information in $\mathbf{X}$ can be used to predict $\mathbf{C}$.
- For fixed $\hat{\boldsymbol{\beta}}$, tuning λ will optimally reduce noise in the predicted probabilities.

Checking the claims

A small example

$n = 9$ variables, square graph.



One predictor plus intercept.

- Small problem.
- Can compute probabilities directly.

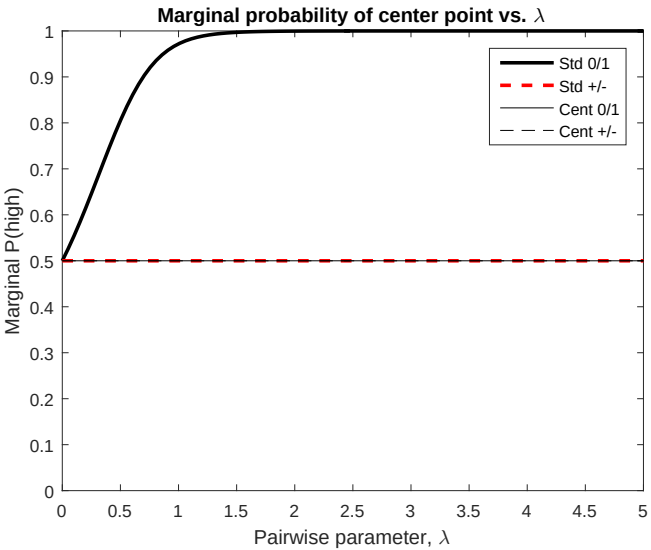
Linear predictor vector is

$$\boldsymbol{\alpha} = \mathbf{X}\boldsymbol{\beta} = \begin{bmatrix} 1 & x_o \\ 1 & x_o \\ 1 & x_o \\ 1 & x_o \\ 1 & x_5 \\ 1 & x_o \\ 1 & x_o \\ 1 & x_o \\ 1 & x_o \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

- Choose values of $x_o, x_5, \beta_0, \beta 1$
- Get marginal $\Pr(C_5 = \text{high})$ as a function of λ, for four models:
  - standard, zero/one
  - standard, plus/minus
  - centered, zero/one
  - centered, plus/minus

Small example: case 1

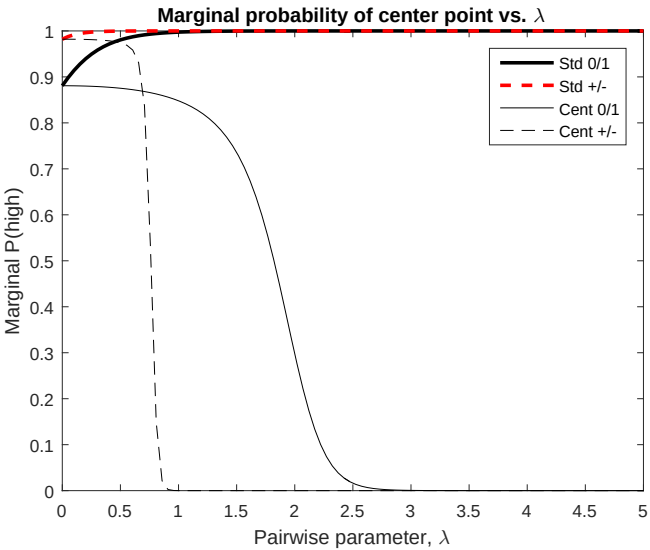
$$\boldsymbol{\beta} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \qquad \text{Linear predictors:} \quad \begin{matrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{matrix}$$



Shows the asymmetry of the standard 0/1 model.

Small example: case 2

$\boldsymbol{\beta} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $x_o = 1$, $x_5 = 1$. Linear predictors: $\begin{matrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{matrix}$

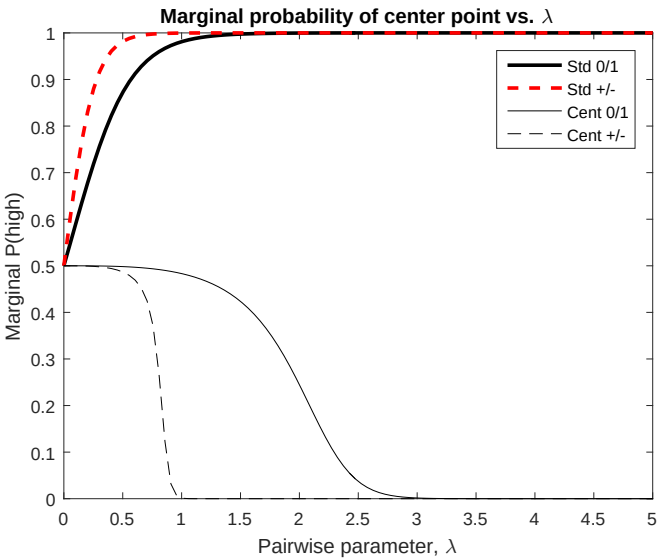


Standard and centered models give opposite behaviour as $\lambda \to \infty$.

Contradicts the idea that centered models have "interpretable parameters."

Small example: case 3

$\boldsymbol{\beta} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $x_o = 1$, $x_5 = -1$. Linear predictors: $\begin{matrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{matrix}$

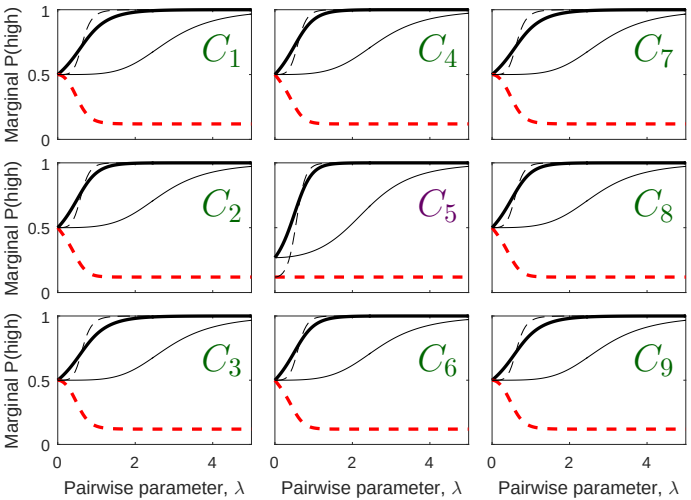


Again, standard and centered models disagree.

Does the centered model behaviour make sense?

Small example: case 4

$\boldsymbol{\beta} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $x_o = 0$, $x_5 = -1$. Linear predictors: $\begin{matrix} 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{matrix}$



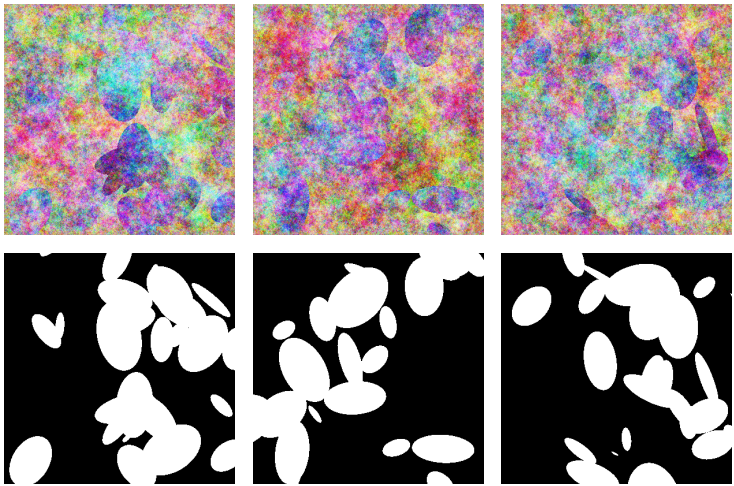
Standard plus/minus very different from the other three.

Limiting probability not equal to 1 or 0.

C_5 probability constant wrt λ.

Simulated images

Generated RGB images with characteristics similar to the smoke data.



- 5 sizes: 100^2, 200^2, 400^2, 600^2 800^2 pixels.
- 90 images at each size.
- training, validation, and test groups.

Simulated images–results 1

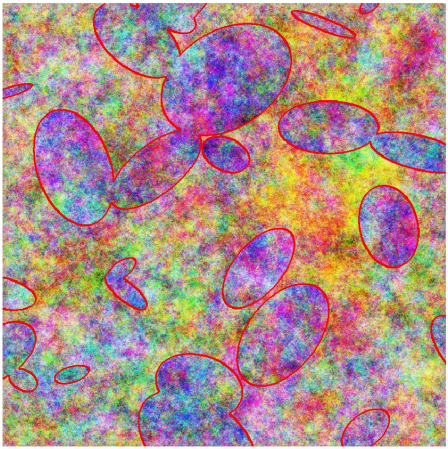
Parameter estimates and prediction error: plug-in vs. pseudolikelihood (plus-minus coding).

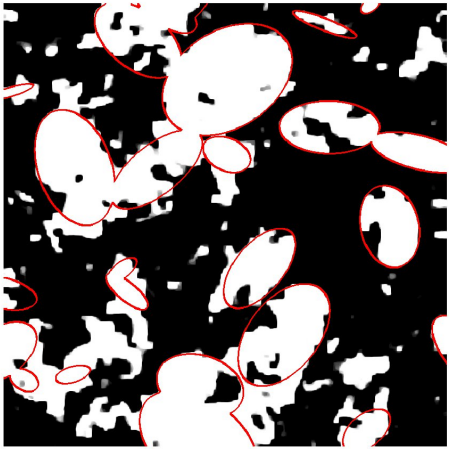
pixels	method	$\hat{R}$	$\hat{G}$	$\hat{B}$	$\hat{\lambda}$	error rate (%)
100^2	plug-in	−2.21	−2.02	1.91	0.90	20.1
	PL	−2.04	−1.99	2.06	0.99	20.4
200^2	plug-in	−1.64	−1.35	1.71	1.00	17.7
	PL	−1.61	−1.30	1.70	1.19	17.7
400^2	plug-in	−2.05	−1.42	1.63	1.60	20.1
	PL	−2.08	−1.40	1.68	1.36	20.1
600^2	plug-in	−1.91	−1.22	1.76	1.95	20.6
	PL	−1.97	−1.36	1.79	1.51	20.4
800^2	plug-in	−1.55	−1.44	1.58	1.95	18.8
	PL	−1.57	−1.43	1.49	1.59	18.6

- Parameter estimates similar.
- Error rates similar.

Simulated images–results 2

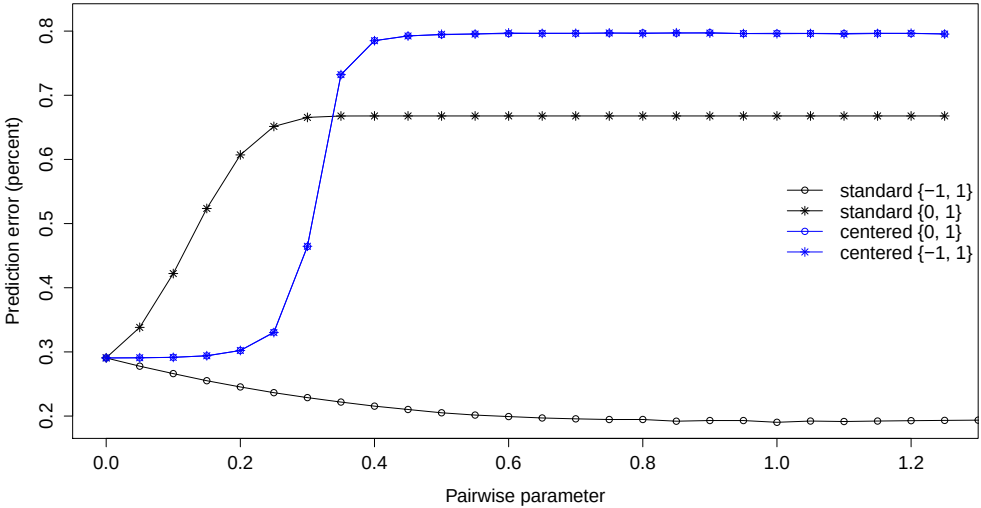
Example predictions, 800×800 image.





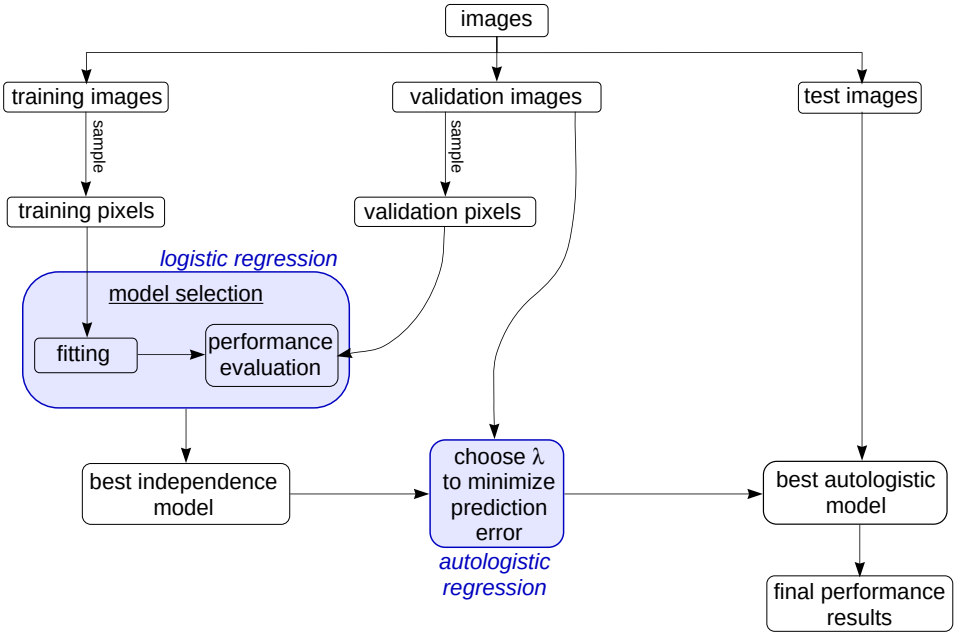
Simulated images–results 3

What about plugin with different model variants?



Analysis of the smoke data

Analysis flowchart



Results 1

Use a logistic GAM

- Each variable or interaction is a piecewise linear function
- Model search by genetic algorithm

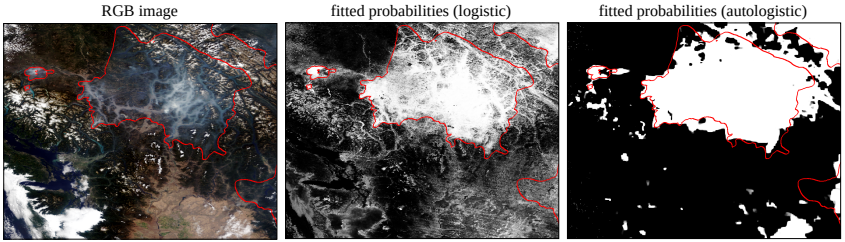
Predictor set	Selected variables (MODIS band numbers)	plug-in $\hat{\lambda}$
main effects	1 6 7 8 14 16 17 18 21 23 25 26 30 31 32 36	1.85
main effects & interactions	7 30 2:3 5:26 6:11 7:36 8:20 8:22 8:25 8:31 13:15 13:23 16:31 18:23 22:36 32:36	1.75

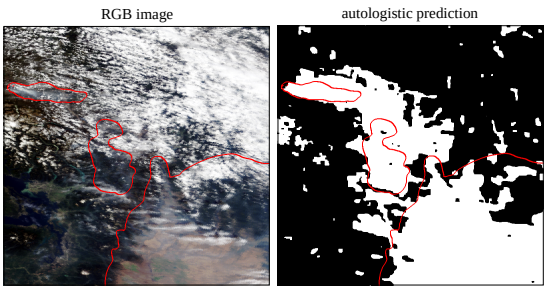
Model	Error rate (%)		
	nonsmoke pixels	smoke pixels	overall
main effects, logistic	21.1	25.9	21.6
interactions, logistic	20.0	23.3	20.3
main effects, autologistic	17.6	23.9	18.2
interactions, autologistic	16.2	21.3	16.7

Results 2

Qualitative results

- Reasonable results in many cases
- Mixed smoke + cloud is still a problem
- Data quality issues (mis-labelled training/test data)





Conclusions and future directions

Summary

- ALR is an interesting option for binary-response regression problems with complex associations.
- Thus far, different communities appear to have used different codings by default.
  - But this yields different models!
  - Plus/minus coding is best?
- The centered model has been put forth as the "new default" ALR model
  - Our work casts doubt on this choice.
- We've proposed a computationally-feasible analysis scheme for ALR with large sets of hyperspectral images.

Further work

- First priority: finish assessments of model variants and formalize
- ALR extensions
  - Let the pairwise parameter be $\lambda(\mathbf{x}_i, \mathbf{x}_j)$: adaptive smoothing.
  - Auto*binomial* model
- Related models
  - MRF of Beta RVs to model probabilities directly?
- Other applications
  - Ecological data
  - Network data
  - . . . suggestions?