Graphical Models and Flexible Classifiers: Bridging the Gap with Boosted Regression Trees

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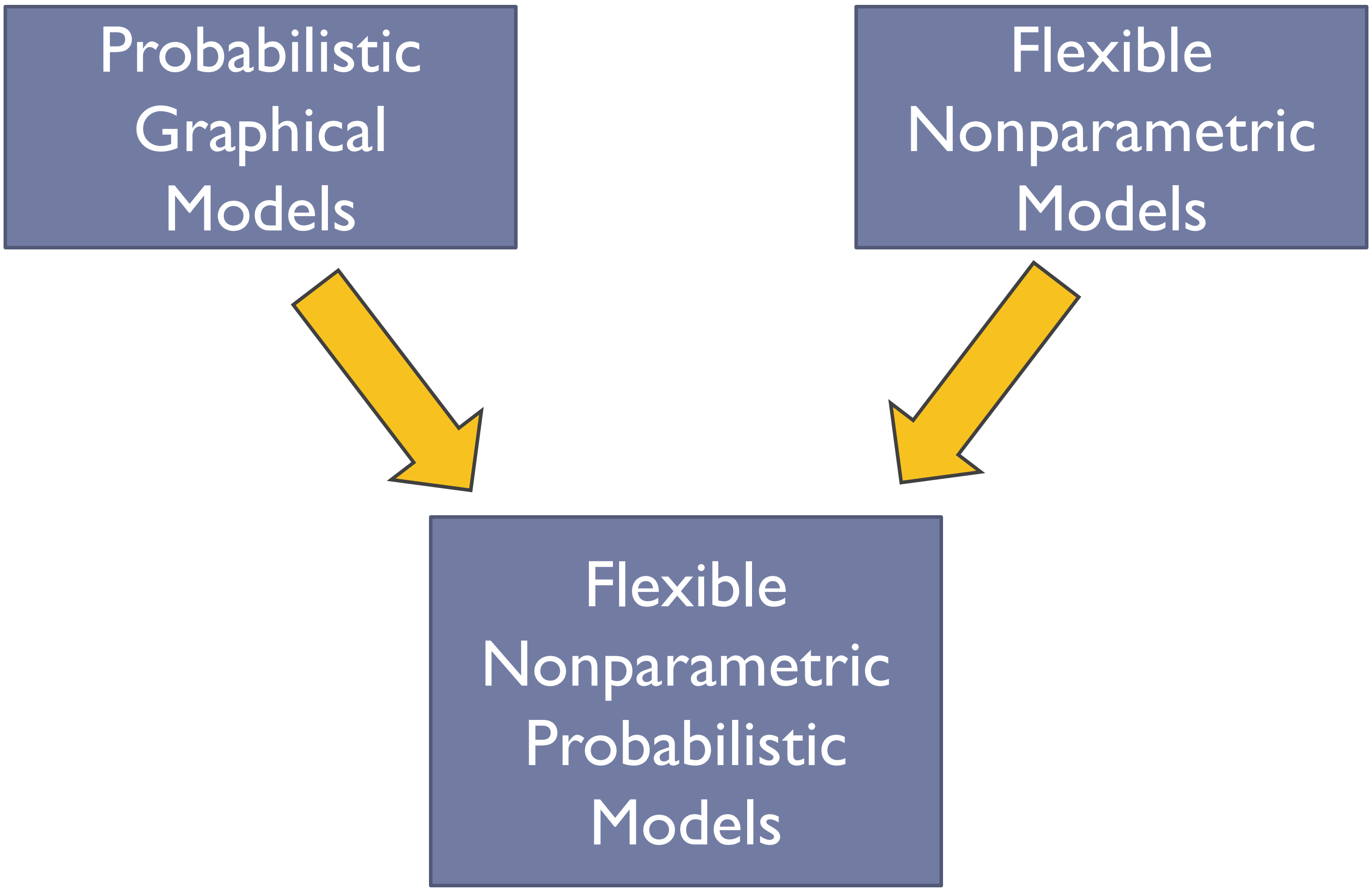
Combining Two Approaches to Machine Learning

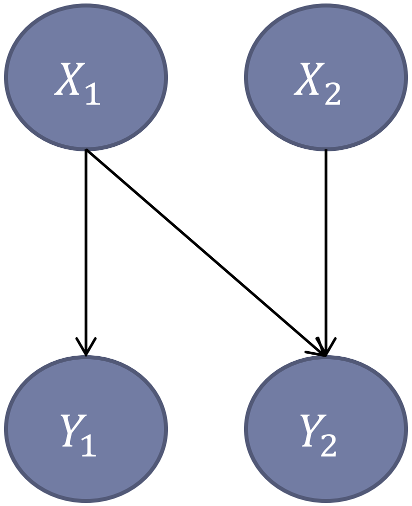


Outline

- Two Cultures of Machine Learning
  - Probabilistic Graphical Models
  - Non-Parametric Discriminative Models
  - Advantages and Disadvantages of Each
- Representing conditional probability distributions using non-parametric machine learning methods
  - Logistic regression (Friedman)
  - Conditional random fields (Dietterich, et al.)
  - Latent variable models (Hutchinson, et al.)
- Ongoing Work
- Conclusions

Probabilistic Graphical Models

- Nodes: Random variables
  - X_1, X_2, Y_1, Y_2
- Edges: Direct probabilistic dependencies
  - $P(Y_1|X_1), P(Y_2|X_1, X_2)$



- Joint probability distribution is the product of the individual node distributions
  - $P(X_1, X_2, Y_1, Y_2) = P(X_1)P(X_2)P(Y_1|X_1)P(Y_2|X_1, X_2)$

Probabilistic Graphical Models (2)

- Can be learned from training data, even when some of the random variables are unobserved (latent or missing)
  - Mixture models (e.g., Gaussian mixture models)
  - Train with EM, gradient descent, or MCMC
- Can represent dynamical processes (Markov models, Dynamic Bayesian Networks)
- Provide probabilistic predictions
  - Useful for integrating into larger systems
- Provide a powerful language for designing and expressing models of complex systems
  - Useful for capturing background knowledge

Probabilistic Graphical Models (3)

- How should the conditional probability distributions be represented?
  - Conditional Probability Tables (CPTs) with one parameter for each combination of values
  - $\frac{2^N}{2}$ parameters

X_1	X_2	Y_1	$P(Y_1 \mid X_1, X_2)$
0	0	0	$1-\alpha$
0	0	1	α
0	1	0	$1-\beta$
0	1	1	β
1	0	0	$1-\gamma$
1	0	1	γ
1	1	0	$1-\delta$
1	1	1	δ

Probabilistic Graphical Models (3)

- How should the conditional probability distributions be represented?
  - Log-linear models (logistic regression)

$$\log \frac{P(Y_1 = 1|X_1, X_2)}{P(Y_1 = 0|X_1, X_2)} =$$

$$\alpha' + I[X_1 = 1]\beta' + I[X_2 = 1]\gamma'$$

  - $\operatorname{expit} u = 1/(1 + \exp(-u))$
  - N parameters

X_1	X_2	Y_1	$P(Y_1\|X_1, X_2)$
0	0	0	$1 - \operatorname{expit} \alpha'$
0	0	1	$\operatorname{expit} \alpha'$
0	1	0	$1 - \operatorname{expit}(\alpha' + \gamma')$
0	1	1	$\operatorname{expit}(\alpha' + \gamma')$
1	0	0	$1 - \operatorname{expit}(\alpha' + \beta')$
1	0	1	$\operatorname{expit}(\alpha' + \beta')$
1	1	0	$1 - \operatorname{expit}(\alpha' + \beta' + \gamma')$
1	1	1	$\operatorname{expit} \alpha' + \beta' + \gamma'$

Advantages and Disadvantages of Parametric Representations

Advantages

- Each parameter has a meaning
- Supports statistical hypothesis testing: "Does X_1 influence Y_1?"
  - $H_0: \beta' = 0$
  - $H_a: \beta' \neq 0$

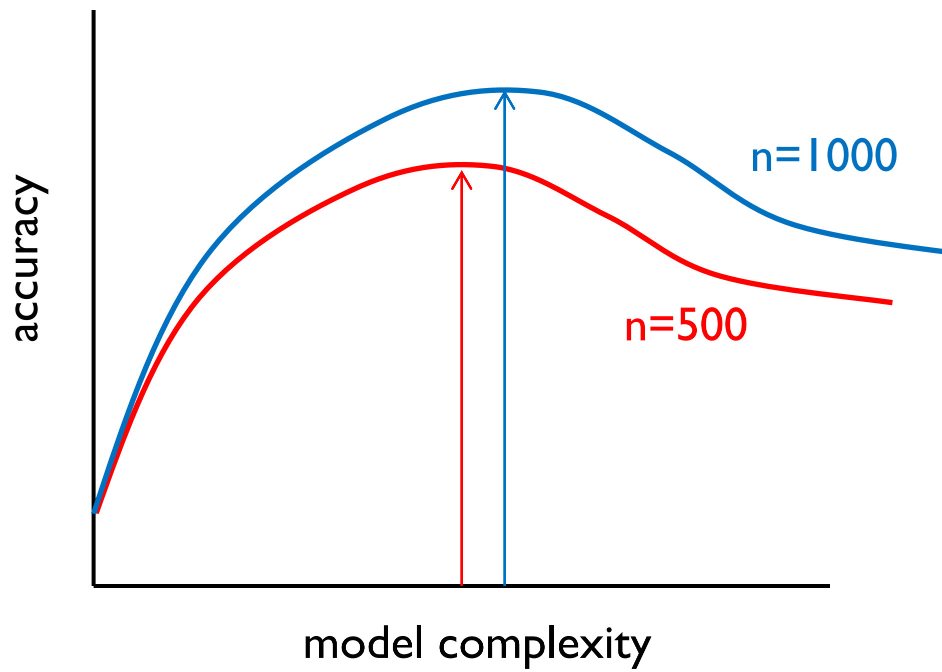
Disadvantages

- Model has fixed complexity
  - Will typically either under-fit or over-fit the data
- Designer must decide about interactions, non-linearities, etc. etc.
  - Wrong decisions lead to highly biased models and invalidate hypothesis tests
  - Correlated variables cause trouble
  - Difficult for problems with many features
- Data must be transformed to match the parametric form
  - Discretized
  - Square root or log transforms

Fundamental Theorem of Statistical Learning

- Three-way tradeoff
  - amount of data
  - complexity of the model
  - prediction accuracy

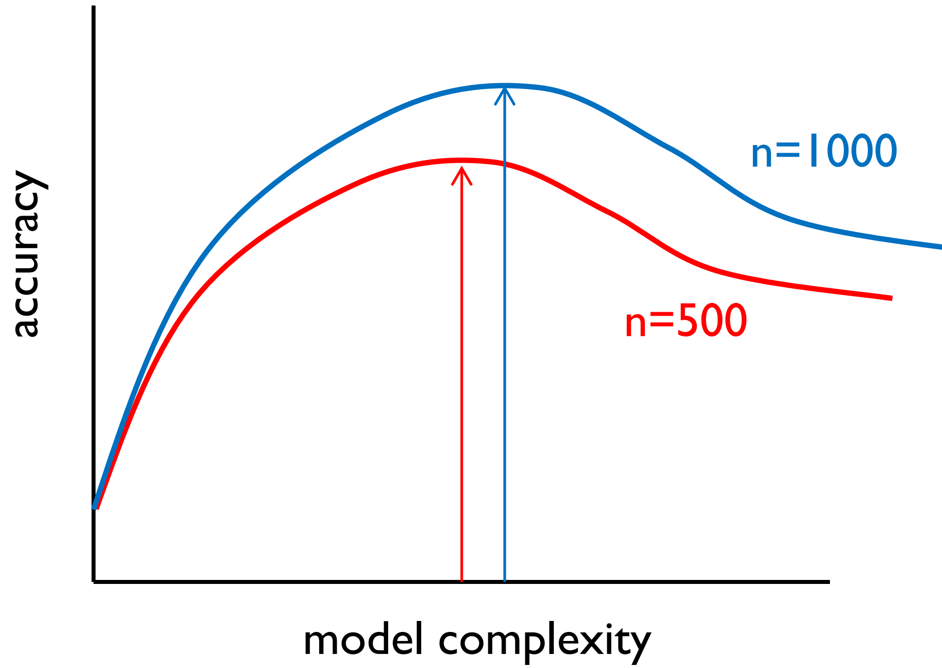
- To achieve optimum accuracy, model complexity should be tuned to the amount of data
  - "Structural Risk Minimization" (Vapnik)



Flexible Machine Learning Models

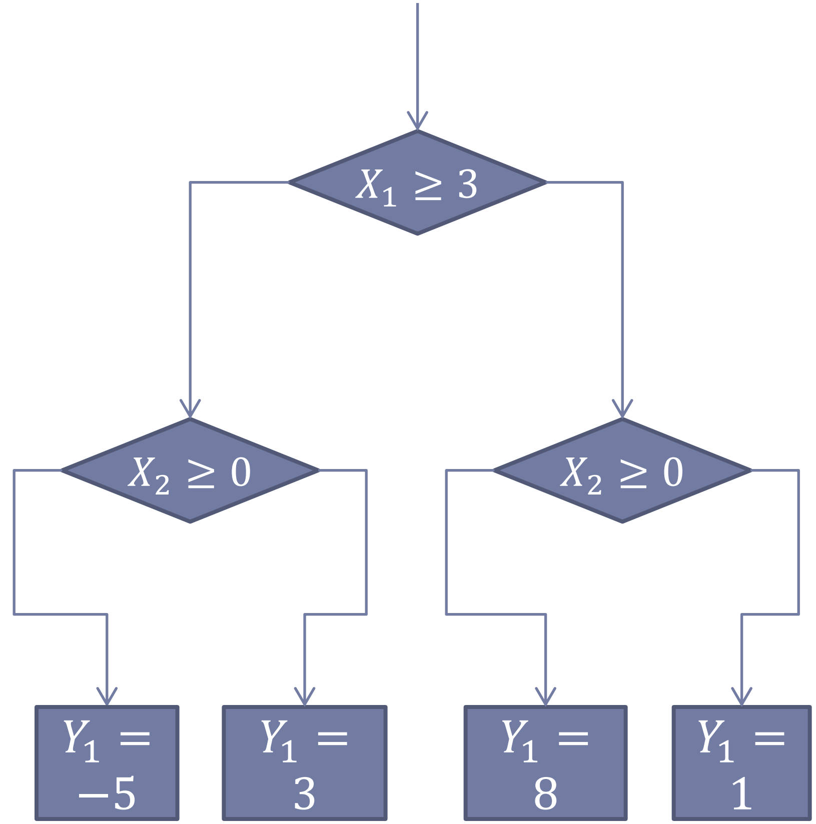
- Support Vector Machines
- Classification and Regression Trees

- Key advantage: Can tune the complexity of the model to the complexity of the data



Another Advantage: Interactions and Nonlinearities

- SVMs:
  - Polynomial kernels capture interactions and polynomial nonlinearities
  - Gaussian kernels capture nonlinearities, however, interactions are embedded in the distance function (typically Euclidean)
- Classification and regression trees
  - Interactions are captured by the if-then-else structure of the tree
  - Nonlinearities are approximated by piecewise constant functions



$$Y_1 = -5 \cdot I(X_1 \geq 3, X_2 \geq 0) + 3 \cdot I(X_1 \geq 3, X_2 < 0) + \\ 8 \cdot I(x_1 < 3, X_2 \geq 0) + 1 \cdot I(X_1 < 3, X_2 < 0)$$

Tree-Based Methods

Advantages

- Flexible Model Complexity
  - Controlled by depth of tree
- Can handle discrete, ordered, and continuous variables
  - No normalization or rescaling needed
- Can handle missing values
  - Proportional distribution
  - Surrogate splits
- Best "off the shelf" method (Breiman)

Disadvantages

- Poor probability estimates
- Do not support hypothesis testing
- Cannot handle latent variables
- High variance, which can be addressed by
  - Boosting
  - Bagging
  - Randomization

Can we combine the best of both?

Probabilistic Graphical Models

- Probabilistic semantics
- Structured by background knowledge
- Latent variables and dynamic processes

Non-Parametric Tree Methods

- Tunable model complexity
- No need for data scaling and preprocessing
  - Discrete, ordered, or continuous values

Existing Efforts

- Dependency Networks
  - Heckerman et al. (JMLR 2000):
    - Bayesian network where each $P(X|Y)$ is a decision tree (with multinomial output probabilities)
  - Trained to maximize pseudo-likelihood
  - Requires all variables to be observed
- RKHS embeddings of probabilities distributions
  - Song, Gretton & Guestrin (AISTATS 2011)
    - Tree-structured graphical model (undirected)
    - No explicit latent variables
- Bayesian semi-parametric methods
  - Dirichlet processes (Blei, Jordan, et al.)

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Representing $P(Y|X)$ using boosted regression trees

- Friedman: Gradient Tree Boosting (2000; Annals of Statistics, 2011)
- Consider logistic regression:
  - $\log \frac{P(Y=1)}{P(Y=0)} = \beta_0 + \beta_1 X_1 + \cdots + \beta_J X_J$
  - $D = \{(X^i, Y^i)\}_{i=1}^N$ are the training examples
  - Log likelihood:
    - $LL(\beta) = \sum_i Y^i \log P(Y = 1|X^i;\beta) + (1 - Y^i) \log P(Y = 0|X^i;\beta)$

Fitting logistic regression via gradient descent

- Let $\beta^0 = g^0 = \mathbf{0}$
- For $\ell = 1, \dots, L$ do
  - Compute $g^\ell = \nabla_\beta LL(\beta)\big|_{\beta=\beta^{\ell-1}}$
    - g^ℓ = gradient w.r.t. β
  - $\beta^\ell := \beta^{\ell-1} + \eta_\ell g^\ell$ take a step of size η_ℓ in direction of gradient
- Final estimate of β is
  - $\beta^L = g^0 + \eta_1 g^1 + \cdots + \eta_L g^L$

Functional Gradient Descent Boosted Regression Trees

- Breiman (1996), Friedman (2000), Mason et al. (NIPS 1999): Fit a logistic regression model as a weighted sum of regression trees:

$$\log \frac{P(Y=1)}{P(Y=0)} = tree^0(X) + \eta_1 tree^1(X) + \cdots + \eta_L tree^L(X)$$

- When "flattened" this gives a log linear model with complex interaction terms

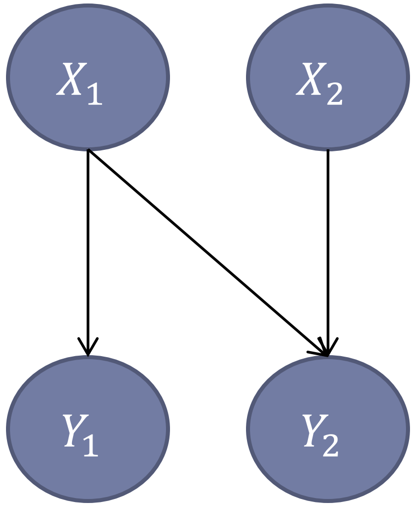
L2-Tree Boosting Algorithm

- Let $F^0(X) = f^0(X) = \mathbf{0}$ be the zero function
- For $\ell = 1, \ldots, L$ do
  - Construct a training set $S^\ell = \{(X^i, \tilde{Y}^i)\}_{i=1}^N$
    - where $\tilde{Y}$ is computed as
    - $\tilde{Y}^i = \left.\frac{\partial LL(F)}{\partial F}\right|_{F=F^{\ell-1}(X^i)}$ // how we wish F would change at X^i
  - Let f^ℓ = regression tree fit to S^ℓ
  - $F^\ell := F^{\ell-1} + \eta_\ell f^\ell$
- The step sizes η_ℓ are the weights computed in boosting
- This provides a general recipe for learning a conditional probability distribution for a Bernoulli or multinomial random variable

L2-TreeBoosting can be applied to any fully-observed directed graphical model

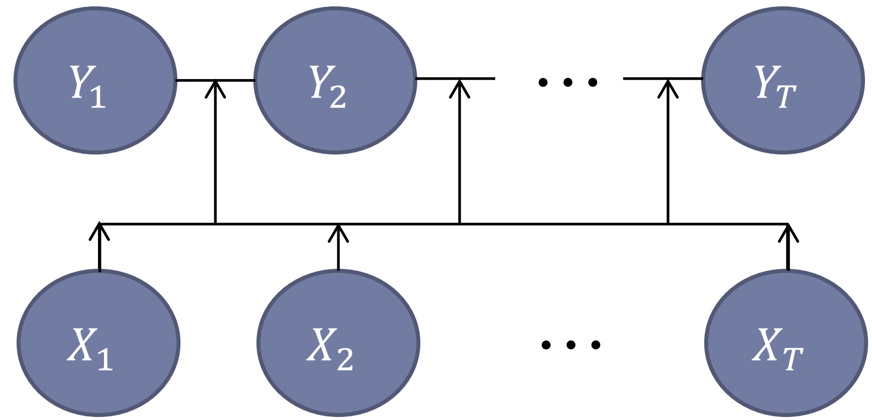
- $P(Y_1|X_1)$ as sum of trees
- $P(Y_2|X_1, X_2)$ as sum of trees

- What about undirected graphical models?



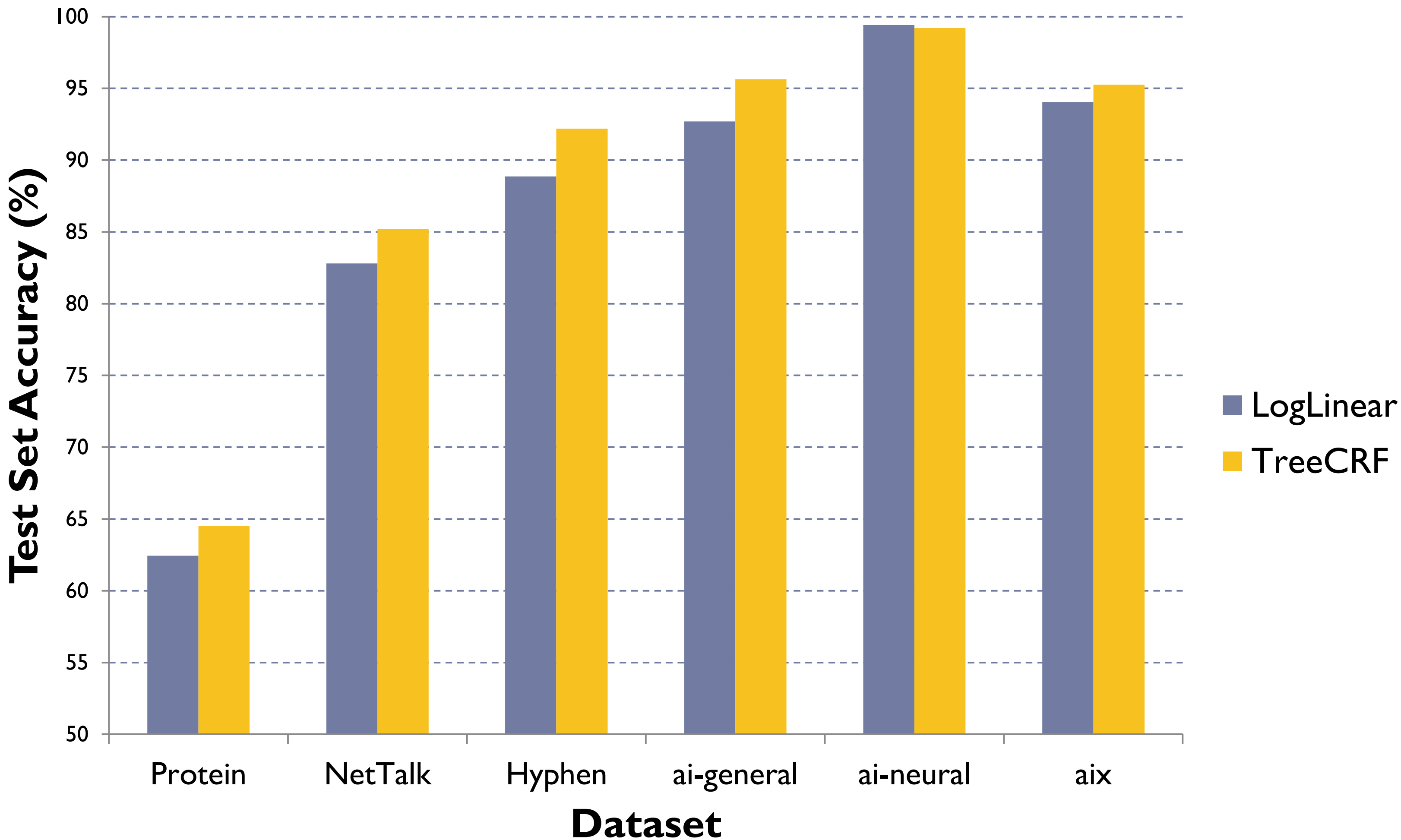
Tree Boosting for Conditional Random Fields

- Conditional Random Field (Lafferty et al., 2001)
  - $P(Y_1, \dots, Y_T | X_1, \dots, X_T)$
  - Undirected graph over the Y's conditioned on the X's.
  - $\Phi(Y_{t-1}, Y_t, X)$ = log linear model



- Dietterich, Hao, Ashenfelter (JMLR 2008; ICML 2004)
  - Fit $\Phi(Y_{t-1}, Y_t, X)$ using tree boosting
  - A form of automatic feature discovery for CRFs

Experimental Results



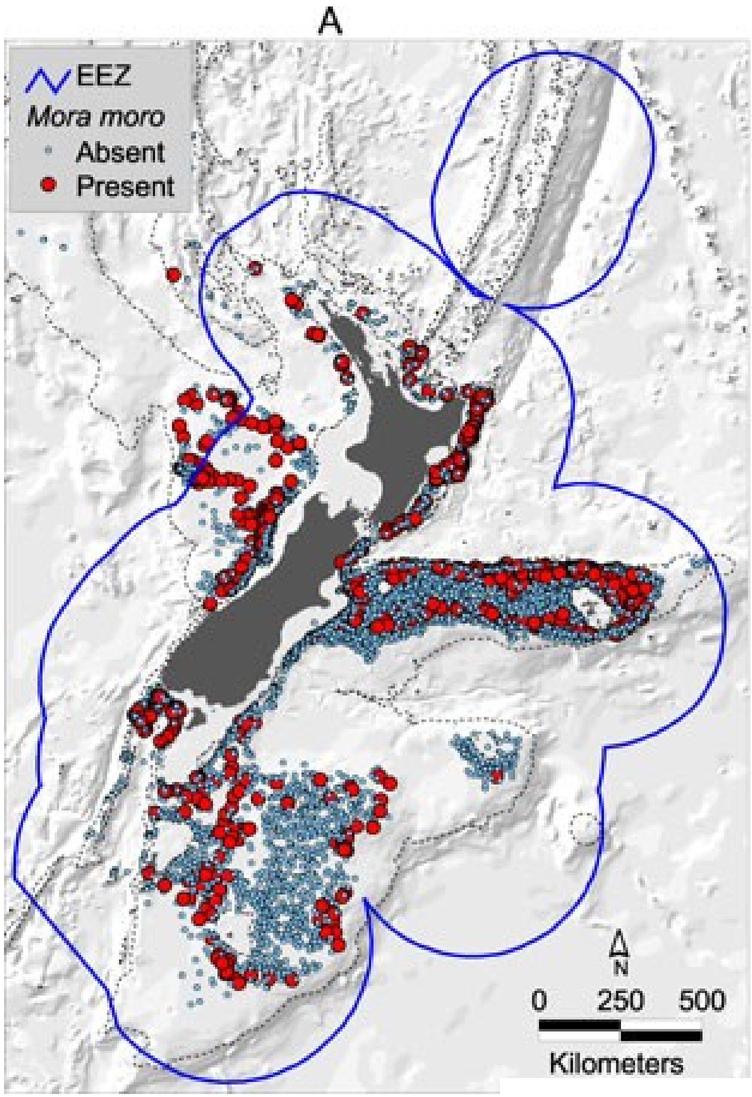
All differences statistically significant $p<0.005$ or better

Tree Boosting for Latent Variable Models

- Both Friedman's L2-TreeBoosted logistic regression and our L2-TreeBoosted CRFs assumed that all variables were observed in the training data
- Can we extend Tree Boosting to <u>latent variable</u> graphical models?
- Motivating application: Species Distribution Modeling

Species Distribution Modeling

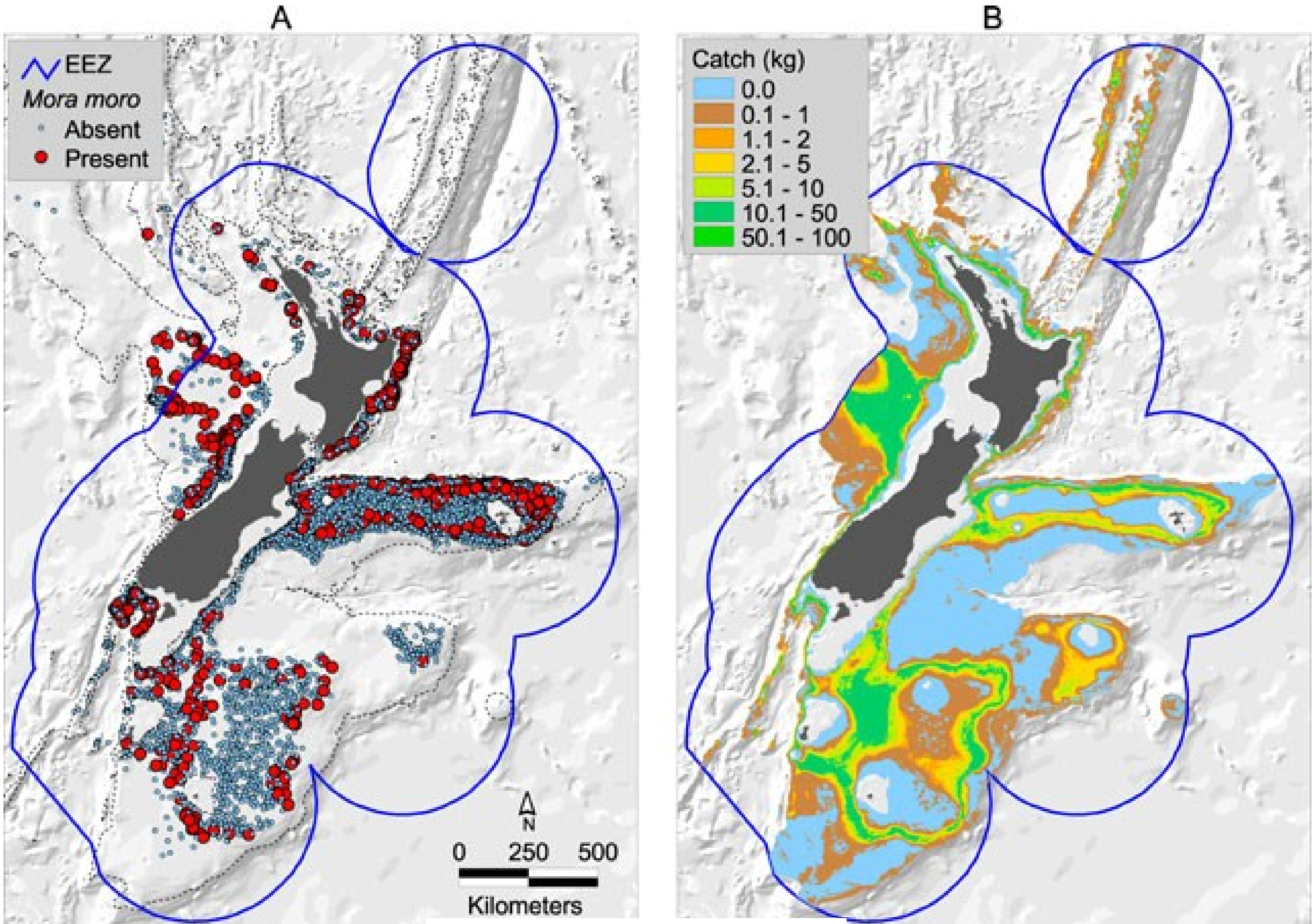
Observations



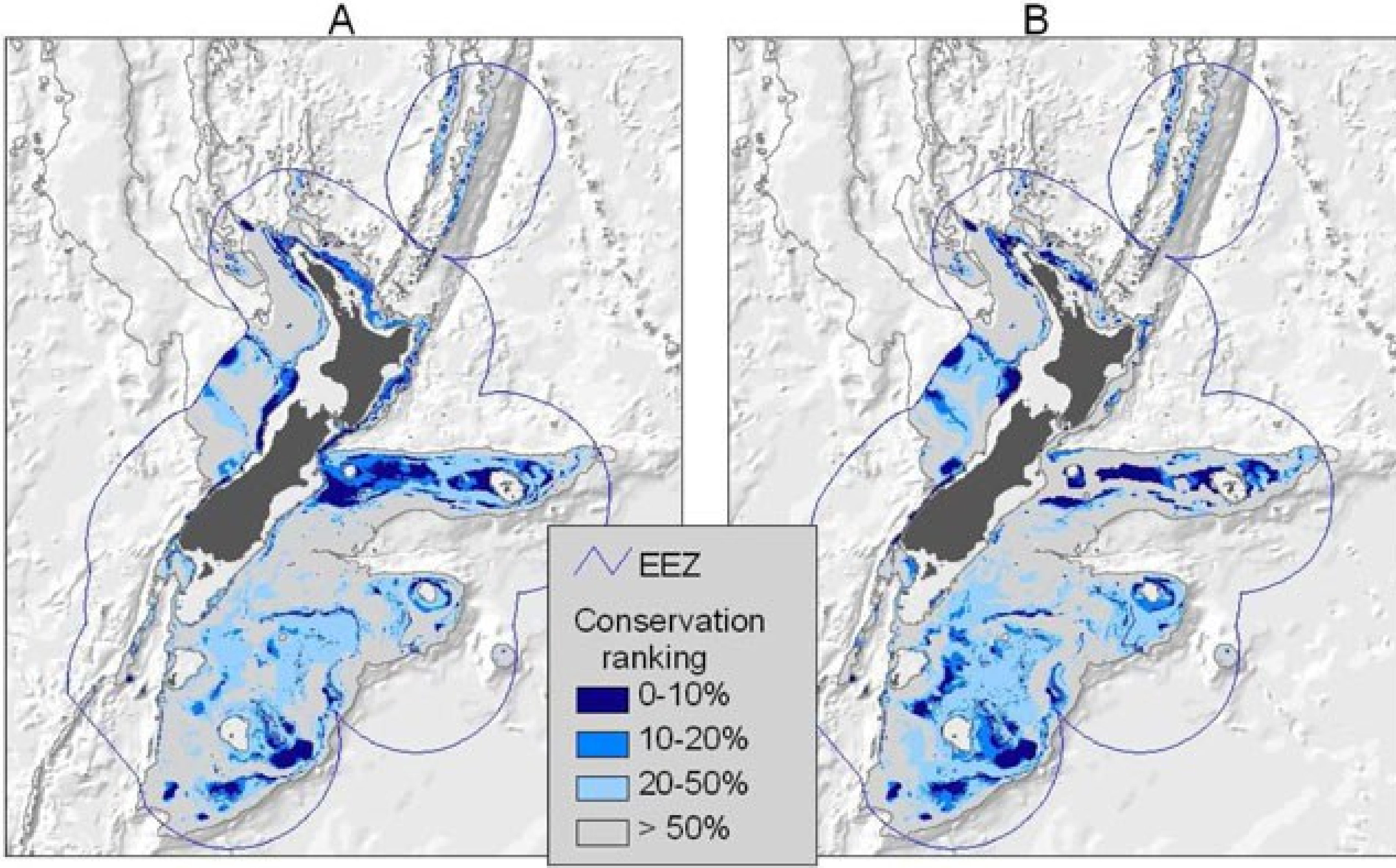
Leathwick et al, 2008

Species Distribution Modeling

Observations | Fitted Model



Leathwick et al, 2008



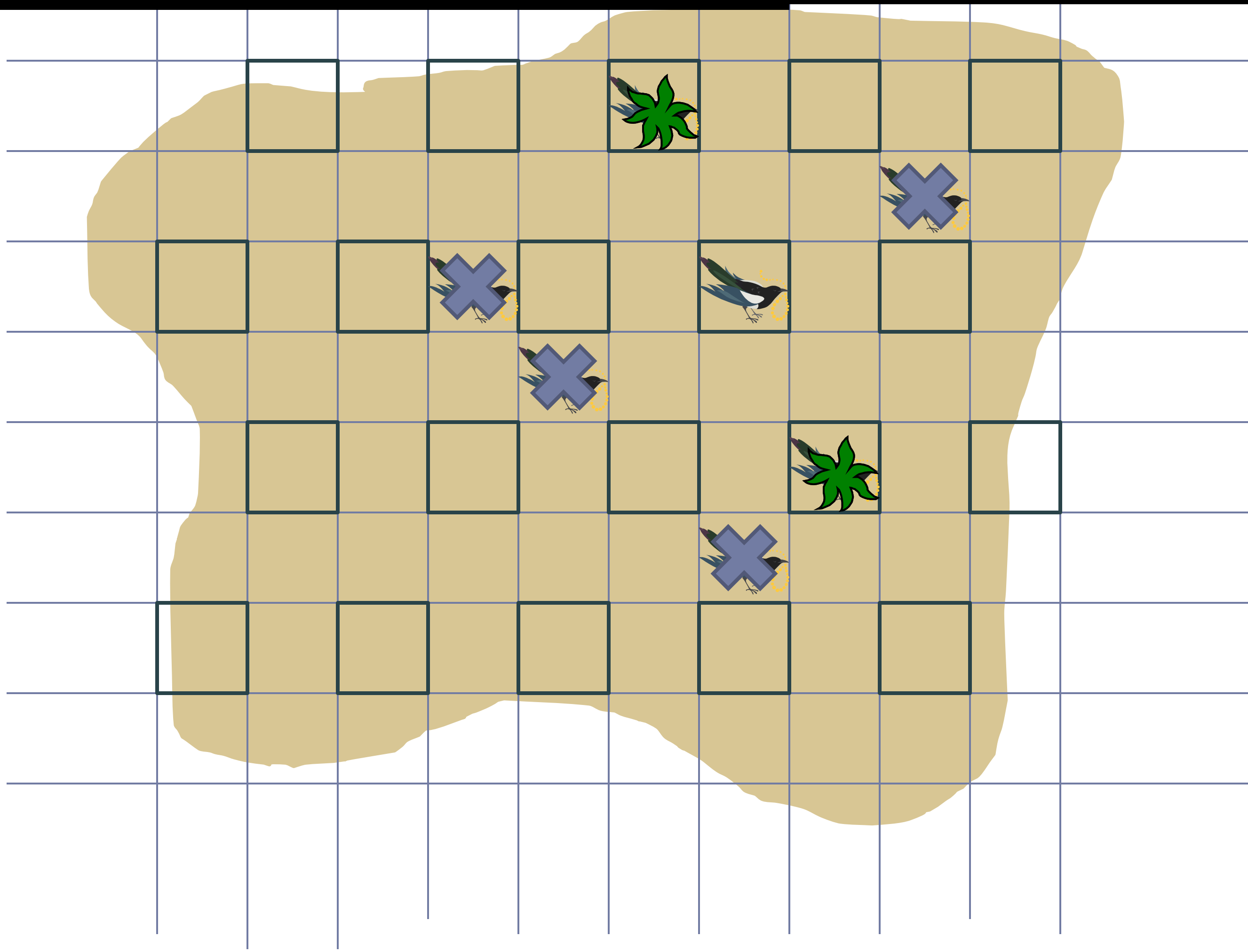
Disregarding costs to fishing industry

Full consideration of costs to fishing industry

Leathwick et al, 2008

Wildlife Surveys with Imperfect Detection

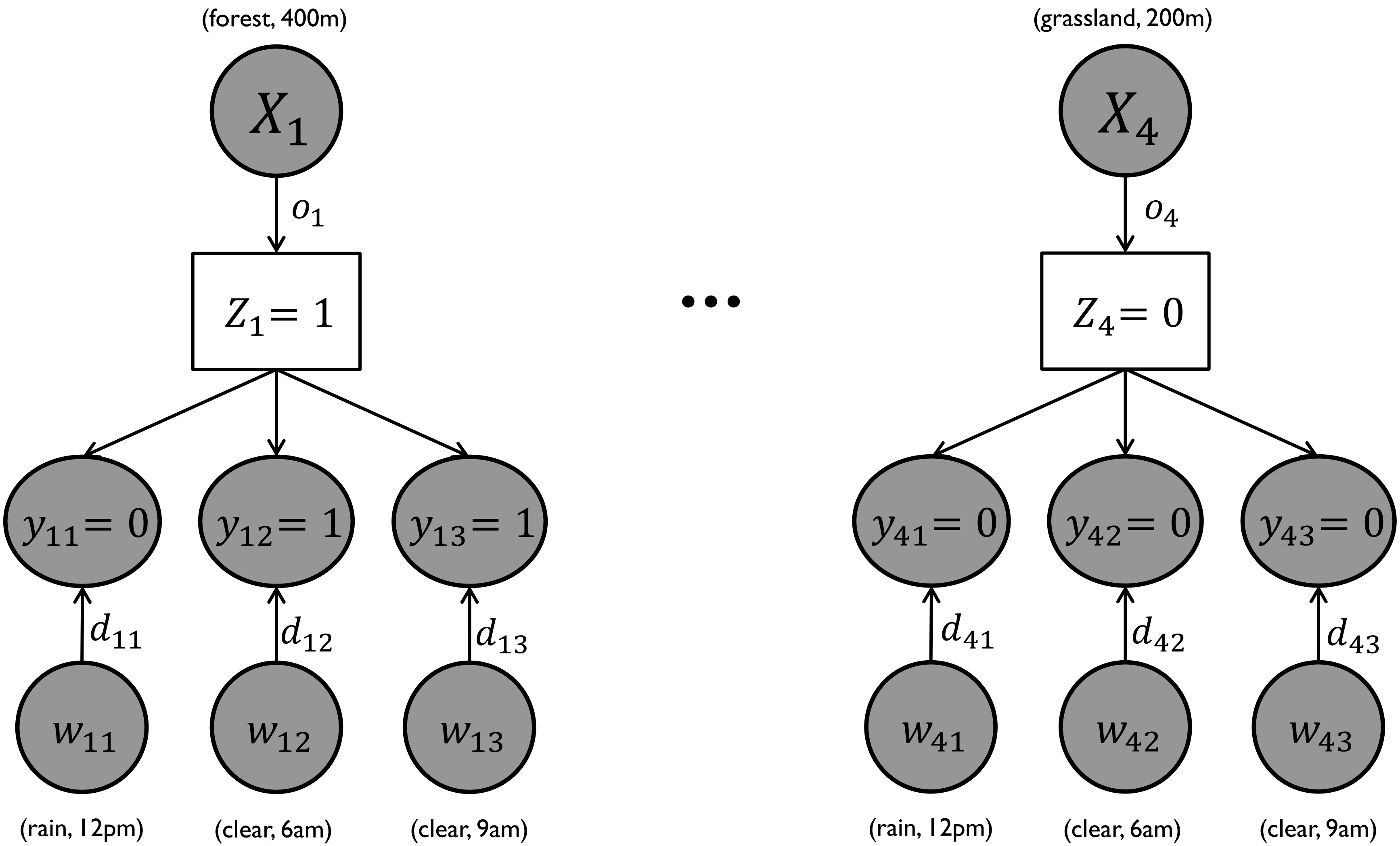
Partial Solution: Multiple visits: Different birds hide on different visits



Multiple Visit Data

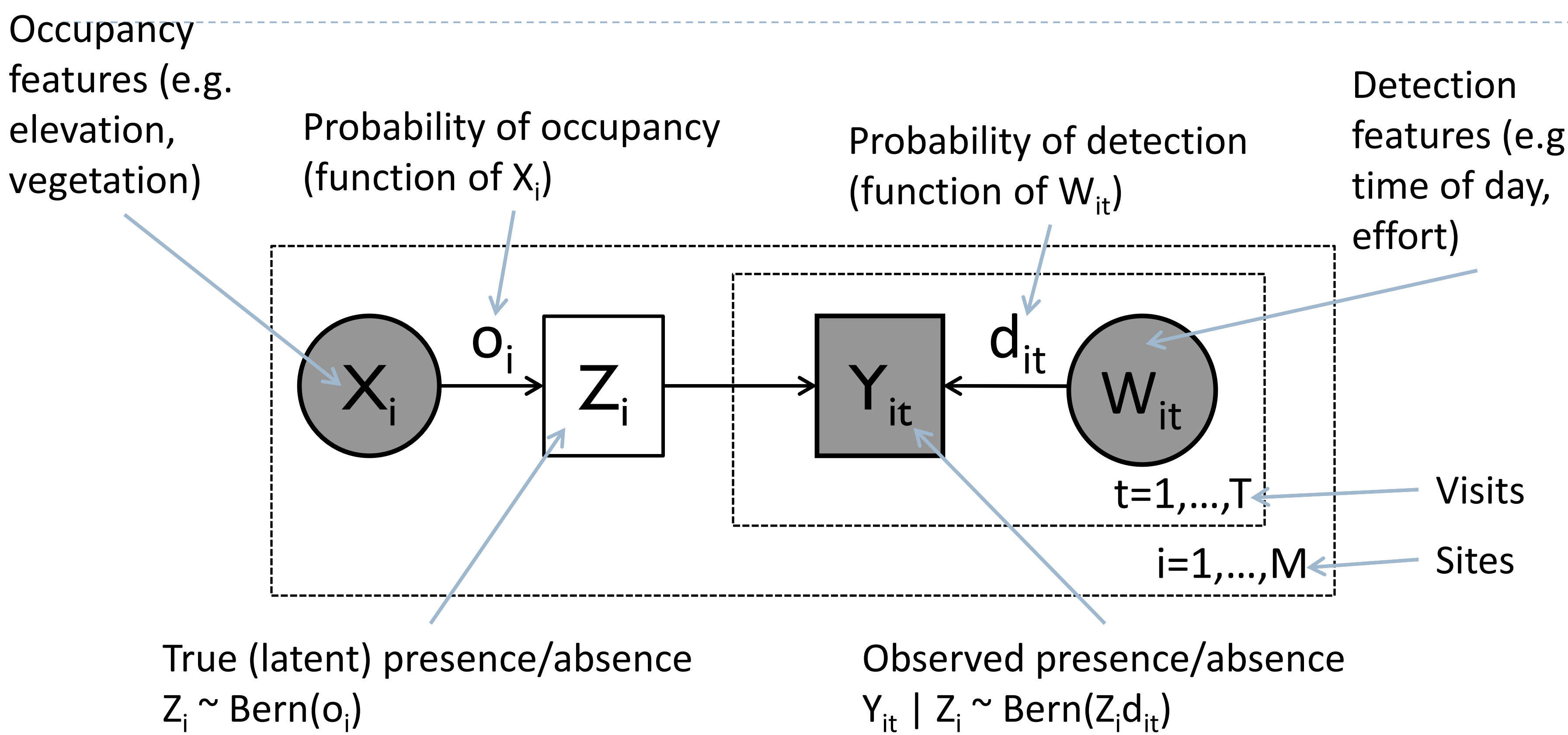
		Detection History		
Site	*True occupancy (latent)*	Visit 1 (rainy day, 12pm)	Visit 2 (clear day, 6am)	Visit 3 (clear day, 9am)
A (forest, elev=400m)	*1*	0	1	1
B (forest, elev=500m)	*1*	0	1	0
C (forest, elev=300m)	*1*	0	0	0
D (grassland, elev=200m)	*0*	0	0	0

Probabilistic Model with Latent Variable Z



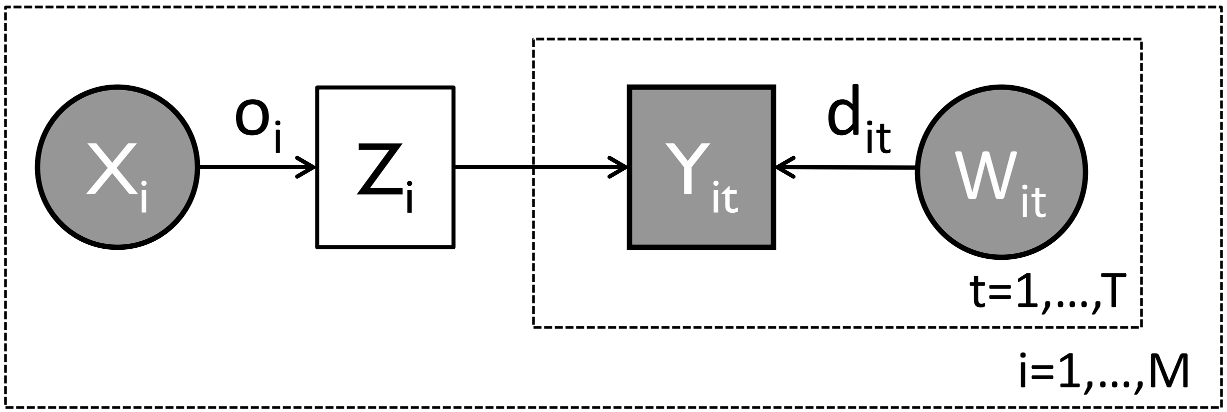
MacKenzie, et al, 2006

Occupancy-Detection Model



MacKenzie, et al, 2006

Parameterizing the model



$z_i \sim P(z_i|x_i)$: Species Distribution Model

$P(z_i = 1|x_i) = o_i = F(x_i)$ "occupancy probability"

$y_{it} \sim P(y_{it}|z_i, w_{it})$: Observation model

$P(y_{it} = 1|z_i, w_{it}) = z_i d_{it}$

$d_{it} = G(w_{it})$ "detection probability"

Standard Approach: Log Linear (logistic regression) models

- $\log \frac{F(X)}{1-F(X)} = \beta_0 + \beta_1 X^1 + \cdots + \beta_J X^J$
- $\log \frac{G(W)}{1-G(W)} = \alpha_0 + \alpha_1 W^1 + \cdots + \alpha_K W^K$
- Train via EM
- People tend to use very simple models: $J = 4, K = 2$

Regression Tree Parameterization

- $\log \frac{F(x)}{1-F(x)} = f^0(x) + \rho_1 f^1(x) + \cdots + \rho_L f^L(x)$
- $\log \frac{G(w)}{1-G(w)} = g^0(w) + \eta_1 g^1(w) + \cdots + \eta_L g^L(w)$
- Perform functional gradient descent on F and G
- Could also use EM

Functional Gradient Descent with Latent Variables

- Loss function $L(F, G, y)$
- $F^0 = G^0 = f^0 = g^0 = 0$
- For $\ell = 1, \dots, L$
  - For each site i compute
    $$\tilde{z}_i = \partial L(F^{\ell-1}(x_i), G^{\ell-1}, y_i) / \partial F^{\ell-1}(x_i)$$
  - Fit regression tree f^ℓ to $\{\langle x_i, \tilde{z}_i \rangle\}_{i=1}^{M}$
  - For each visit t to site i, compute
    $$\tilde{y}_{it} = \partial L\left(F^{\ell-1}(x_i), G^{\ell-1}(w_{it}), y_{it}\right) / \partial G^{\ell-1}(w_{it})$$
  - Fit regression tree g^ℓ to $\{\langle w_{it}, \tilde{y}_{it} \rangle\}_{i=1,t=1}^{M,T_i}$
  - Let $F^\ell = F^{\ell-1} + \rho_\ell f^\ell$
  - Let $G^\ell = G^{\ell-1} + \eta_\ell g^\ell$

Experiment

- Algorithms:
  - Supervised methods:
    - S-LR: logistic regression from $(x_i, w_{it}) \rightarrow y_{it}$
    - S-BRT: boosted regression trees $(x_i, w_{it}) \rightarrow y_{it}$
  - Occupancy-Detection methods:
    - OD-LR: F and G logistic regressions
    - OD-BRT: F and G boosted regression trees
- Data:
  - 12 bird species
  - 3 synthetic species
  - 3124 observations from New York State, May-July 2006-2008
  - All features rescaled to zero mean, unit variance

Features

$X^{(1)}$	Human population per sq. mile
$X^{(2)}$	Number of housing units per sq. mile
$X^{(3)}$	Percentage of housing units vacant
$X^{(4)}$	Elevation
$X^{(5)} \ldots X^{(19)}$	Percent of surrounding 22,500 hectares in each of 15 habitat classes from the National Land Cover Dataset
$W^{(1)}$	Time of day
$W^{(2)}$	Observation duration
$W^{(3)}$	Distance traveled during observation
$W^{(4)}$	Day of year

Simulation Study using Synthetic Species

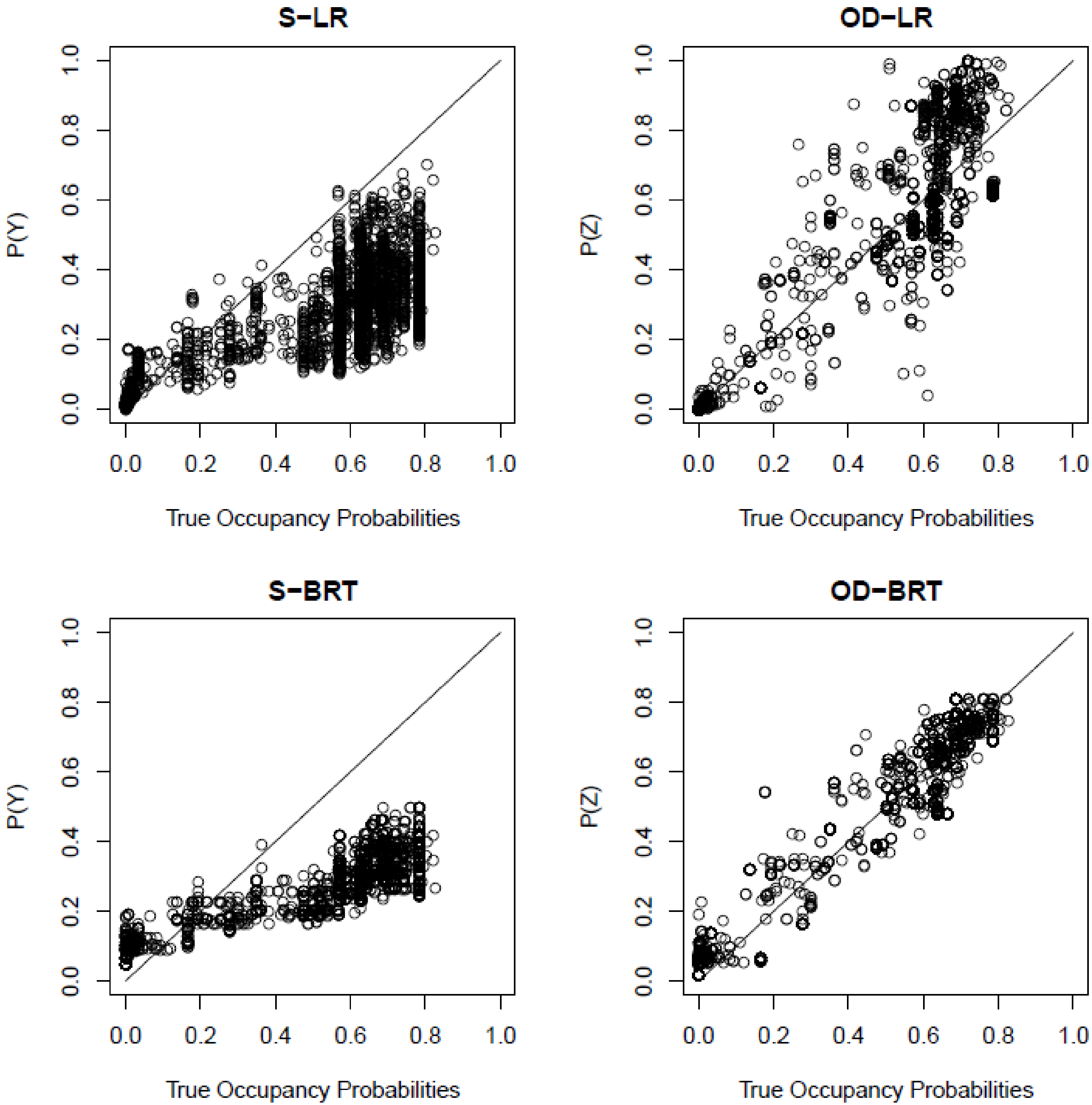
- Synthetic Species 2: F and G nonlinear

$$\log\frac{o_i}{1-o_i} = -2\left[x_i^{(1)}\right]^2 + 3\left[x_i^{(2)}\right]^2 - 2x_i^{(3)}$$

$$\log\frac{d_{it}}{1-d_{it}} = \exp(-0.5w_{it}^{(4)}) + \sin(1.25w_{it}^{(1)} + 5)$$

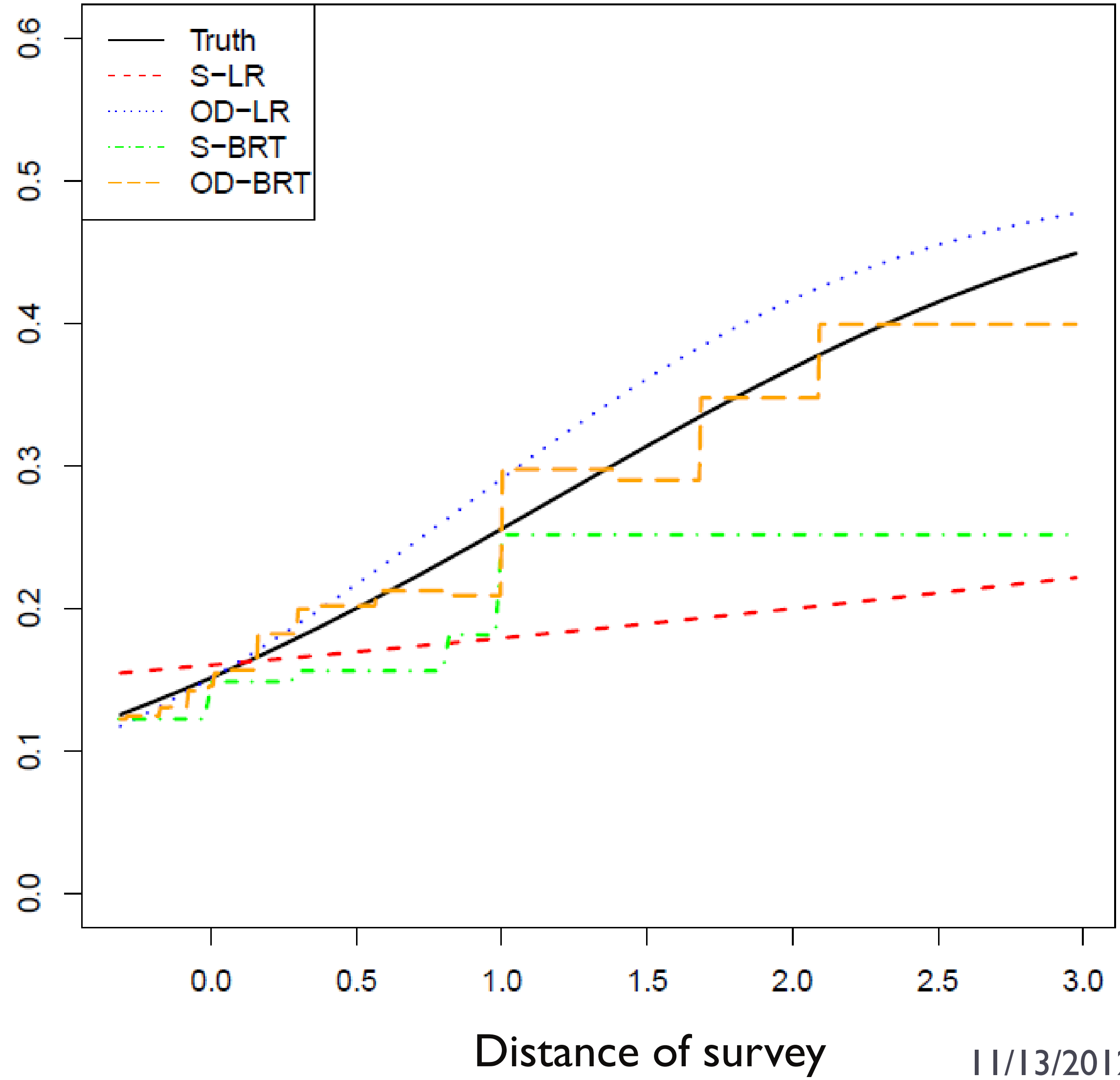
Predicting Occupancy

Synthetic Species 2



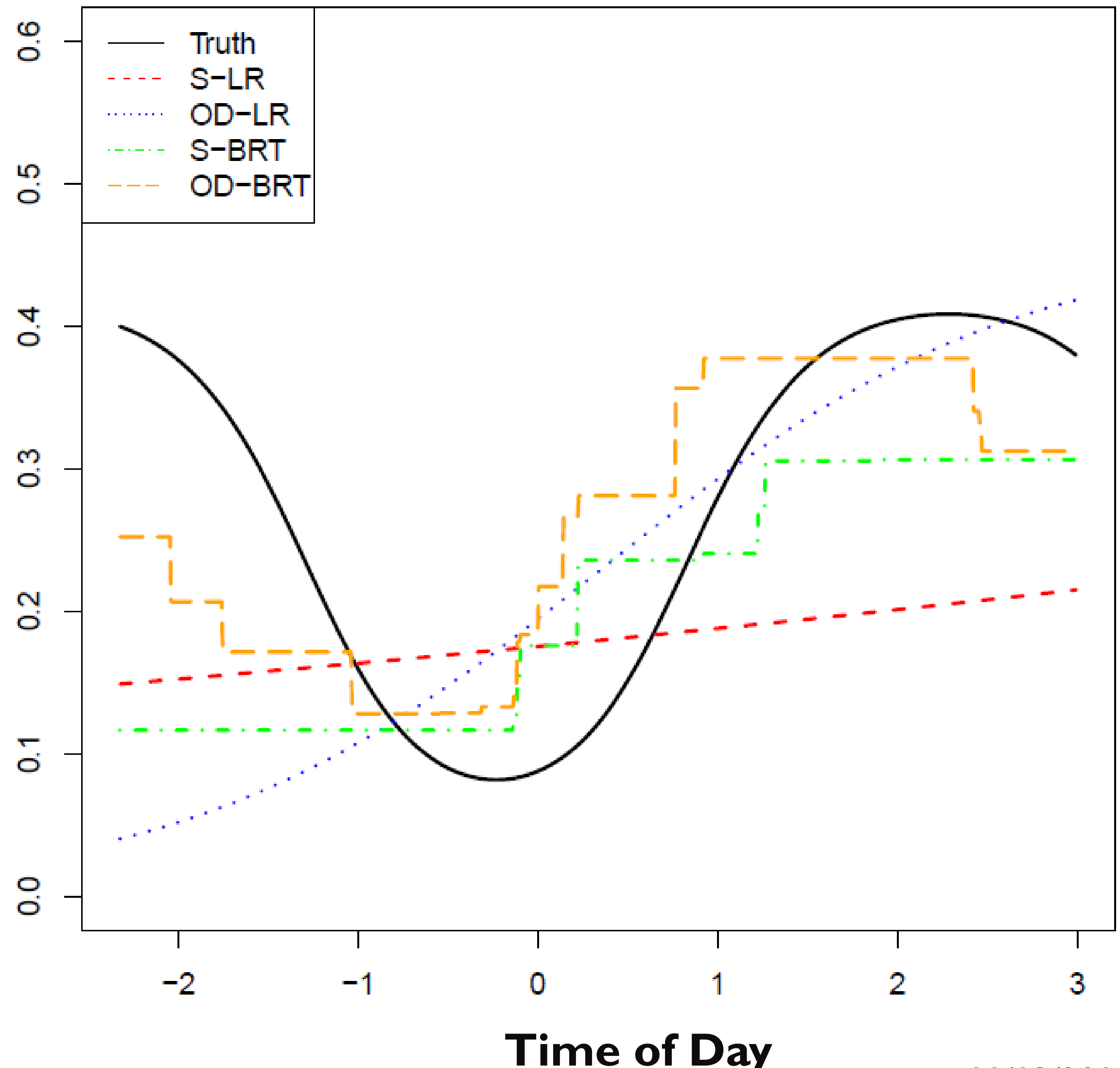
Partial Dependence Plot
Synthetic Species 1

- OD-BRT has the least bias

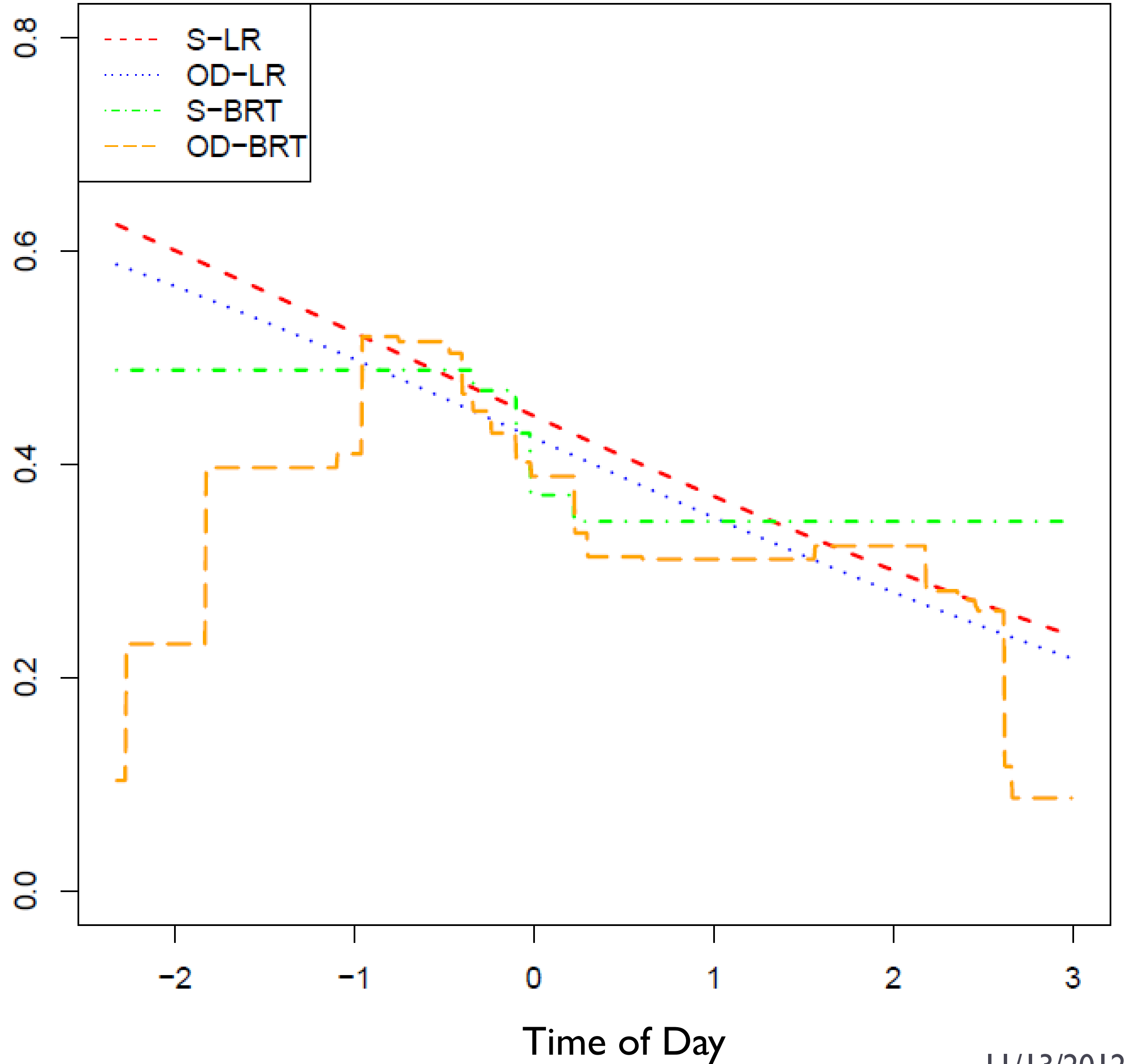


Partial Dependence Plot
Synthetic Species 3

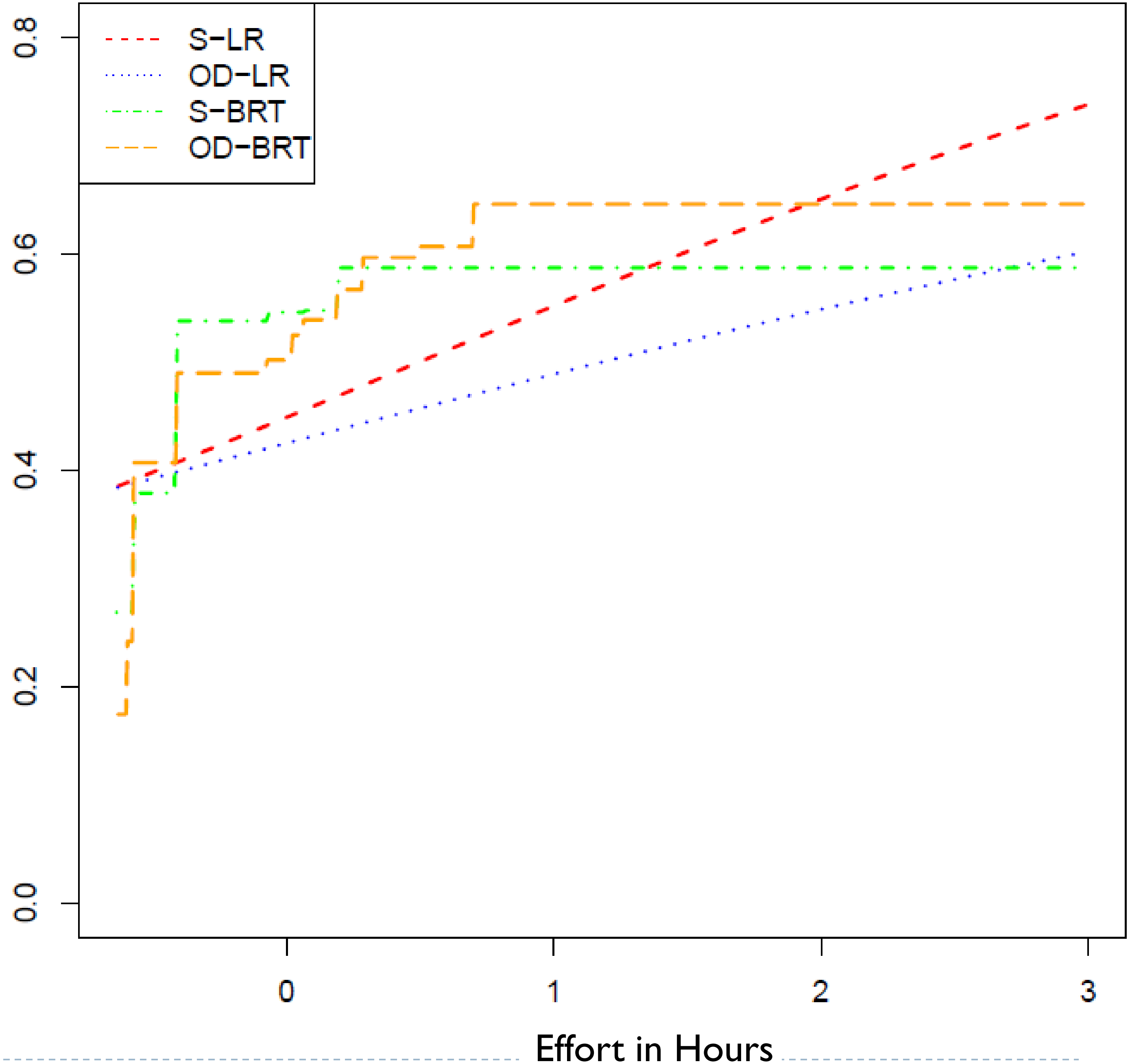
- OD-BRT has the least bias and correctly captures the bi-modal detection probability



Partial Dependence Plot Blue Jay vs. Time of Day



Partial Dependence Plot Blue Jay vs. Duration of Observation



Open Problems

- Sometimes the OD model finds trivial solutions
  - Detection probability = 0 at many sites, which allows the Occupancy model complete freedom at those sites
  - Occupancy probability constant (0.2)
- Log likelihood for latent variable models suffers from local minima
  - Proper initialization?
  - Proper regularization?
  - Posterior regularization?
- How much data do we need to fit this model?
  - Can we detect when the model has failed?

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Next Steps

- Modeling Expertise in Citizen Science
- From Occupancy (0/1) to Abundance (n)
- From Static to Dynamic Models

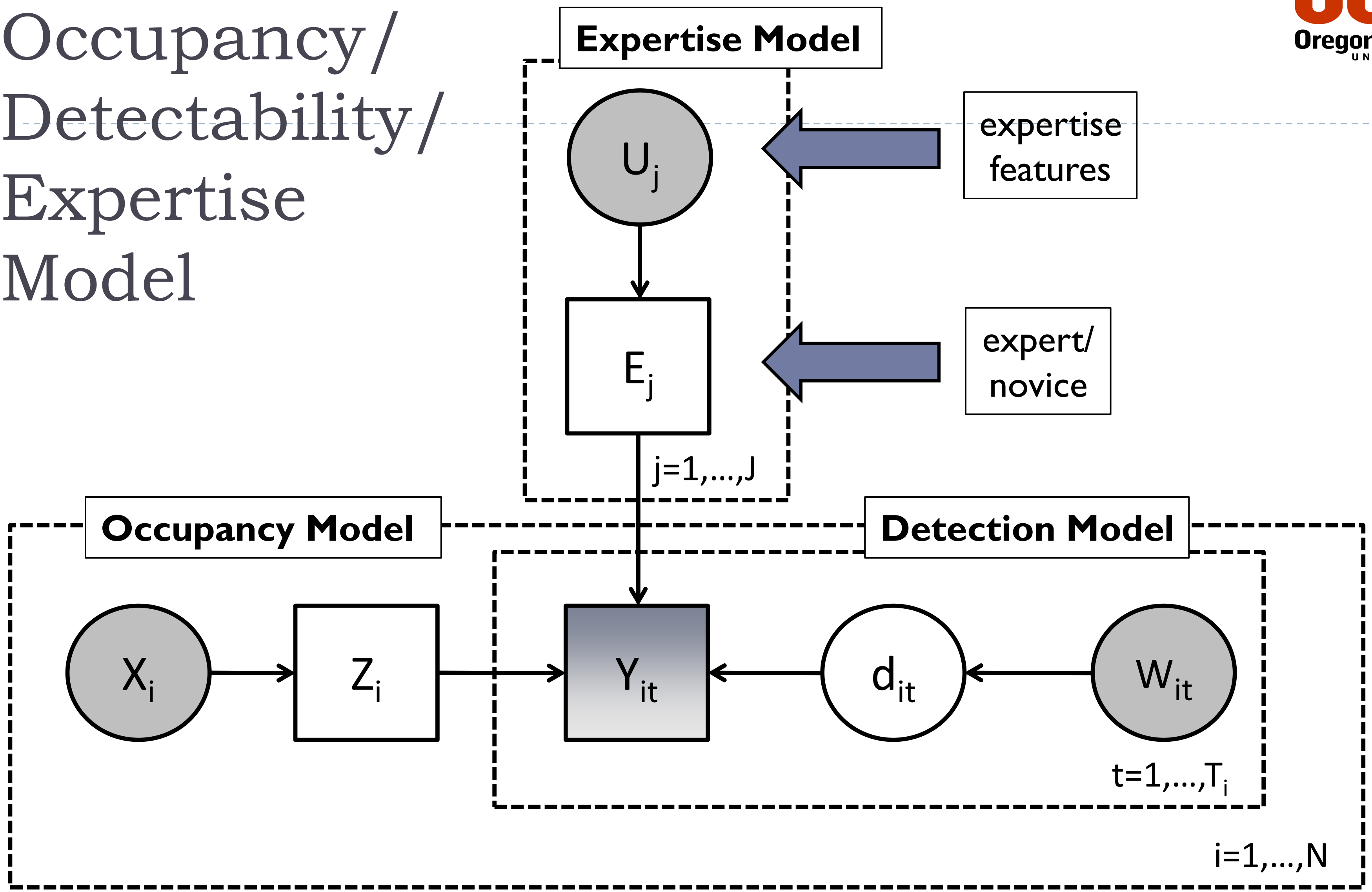
Modeling Expertise in Citizen Science

- Project eBird
  - Bird watchers upload checklists to ebird.org
  - 8,000-12,000 checklists per day uploaded
  - World-wide coverage 24x365
  - 38,599 observers; 336,088 locations
  - 2.4M checklists; 41.7M observations
  - All bird species (~3,000)

  - [Please volunteer! We need more observers in S.America]

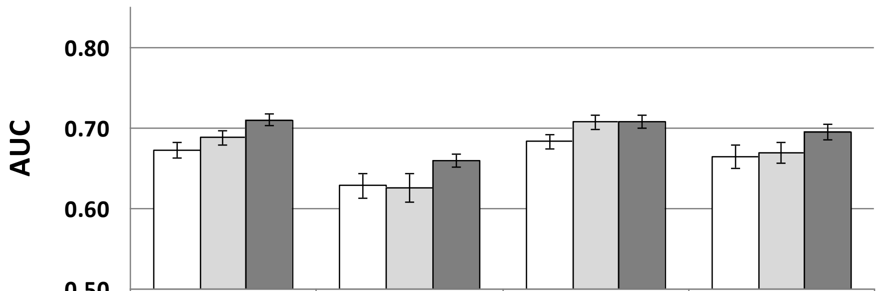
- Wide variation in "birder" expertise

Occupancy/ Detectability/ Expertise Model



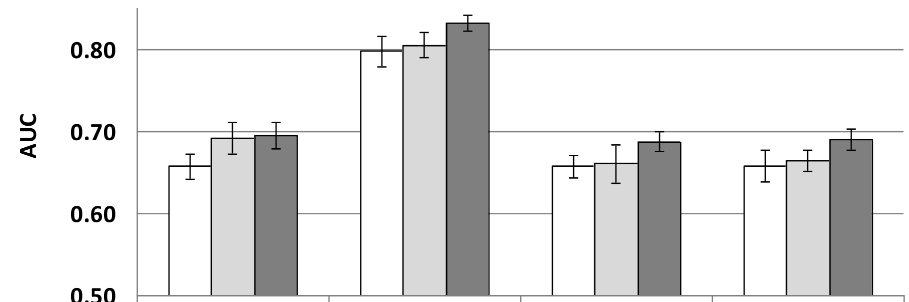
First Results

Average AUC on four common bird species



	Blue Jay	White-breasted Nuthatch	Northern Cardinal	Great Blue Heron
LR	0.6726	0.6283	0.6831	0.6641
OD	0.6881	0.6262	0.7073	0.6691
ODE	0.7104	0.6600	0.7085	0.6959

Average AUC on four hard-to-detect bird species



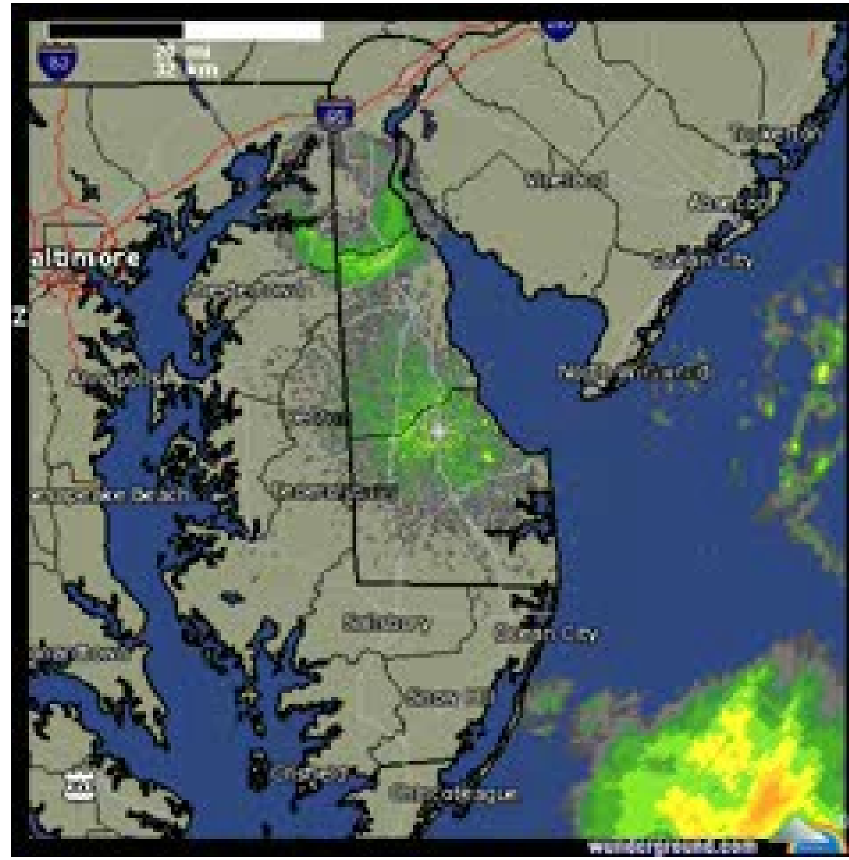
	Brown Thrasher	Blue-headed Vireo	Northern Rough-winged Swallow	Wood Thrush
LR	0.6576	0.7976	0.6575	0.6579
OD	0.6920	0.8055	0.6609	0.6643
ODE	0.6954	0.8325	0.6872	0.6903

- eBird data for May and June (peak detectability period) for NYState
- Expertise component trained via supervised learning

Jun Yu, Weng-Keen Wong, Rebecca Hutchinson (2010). *Modeling Experts and Novices in Citizen Science Data*. ICDM 2010.

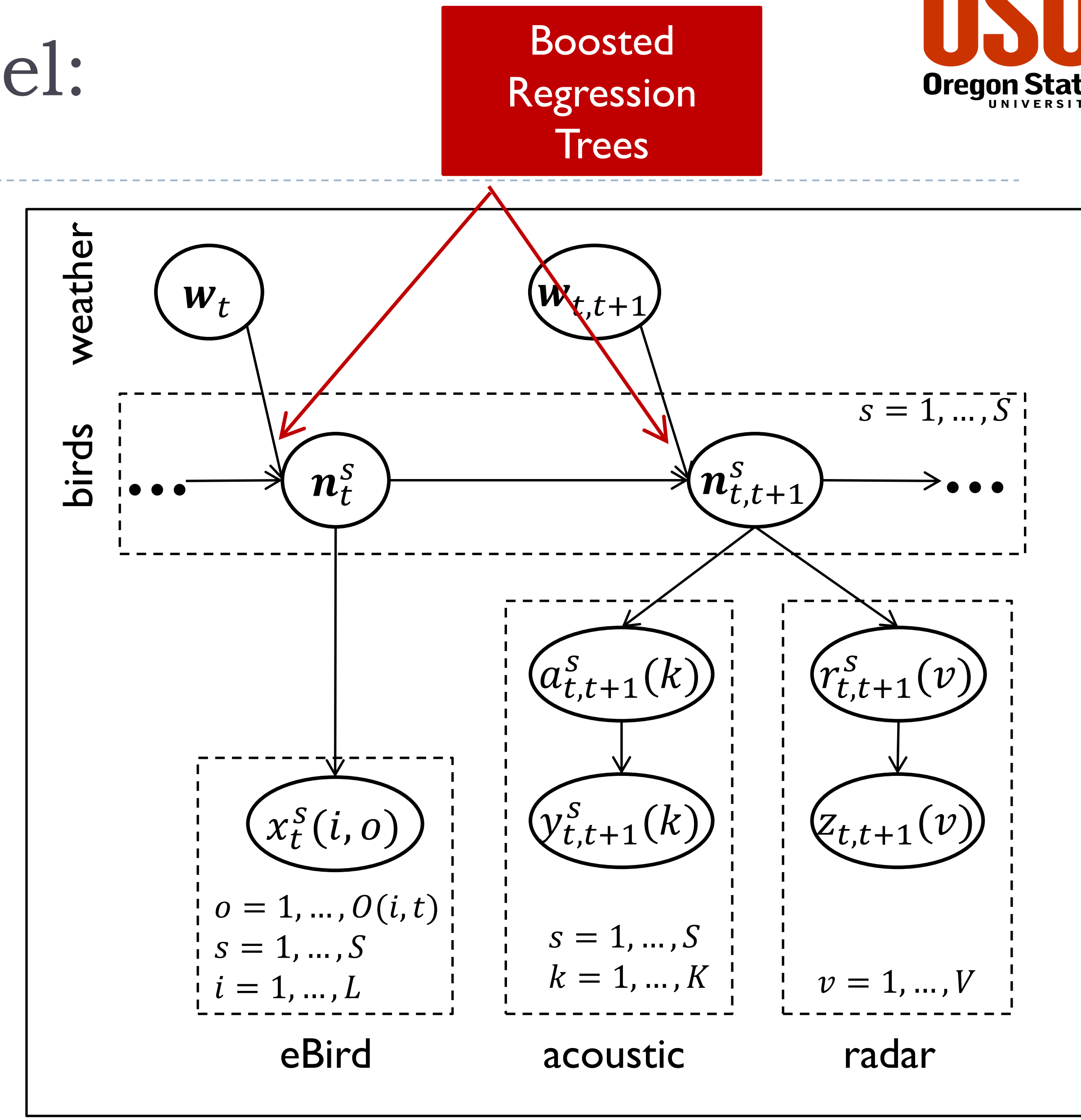
New Project: BirdCast

- Goal: Continent-wide bird migration forecasting
- Additional data sources:
  - Doppler weather radar
  - Night flight calls
  - Wind observations (assimilated to wind forecast model)



BirdCast Model:

- $n_t^s(c)$ = # of birds of species s at cell c and time t.
- $\boldsymbol{w}_t$ = weather variables (wind, temperature, precipitation)
- $x_t^s(i,o)$ = eBird count for visit o at site i species s and time t
- $y_{t,t+1}^s(k)$ = # of flight calls for species s at site k on the night $(t, t+1)$
- $z_{t,t+1}$ = # of birds (all species) observed at radar v on night $(t, t+1)$
- Occupancy changes each night



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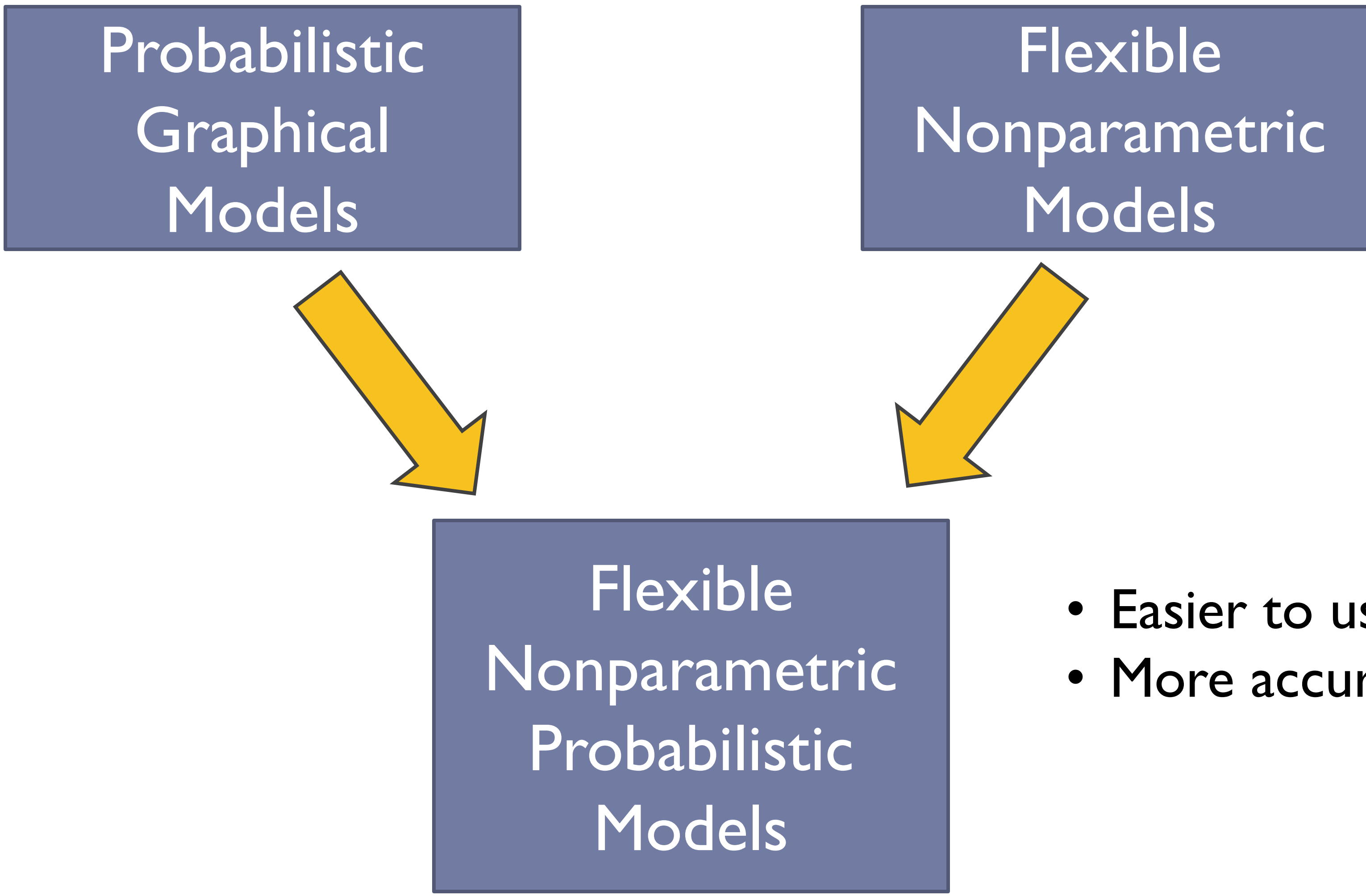
Concluding Remarks

- Gradient Tree Boosting can be integrated into probabilistic graphical models
  - Fully-observed directed models
  - Conditional random fields
  - Latent variable models
- When to do this?
  - When you want to condition on a large number of features
  - When you have a lot of data

Combining Two Approaches to Machine Learning



- Easier to use
- More accurate

Thank-you

- Adam Ashenfelter, Guo-Hua Hao: TreeBoosting for CRFs
- Rebecca Hutchinson, Liping Liu: Boosted Regression Trees in OD models
- Weng-Keen Wong, Jun Yu: ODE model
- Dan Sheldon: Models for Bird Migration
- Steve Kelling and colleagues at the Cornell Lab of Ornithology

- National Science Foundation Grants 0083292, 0307592, 0832804, and 0905885