# Mondrian Forests

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# Outline

Motivation and Background

Mondrian Forests
- Randomization mechanism
- Online training
- Prediction and Hierarchical smoothing
- Classification Experiments: online vs batch
- Regression Experiments: evaluating uncertainty estimates

Conclusion

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Lots of neat ideas in Bayesian non-parametrics; can we use these in a non-Bayesian context?

# Problem setup

- **Input**: attributes $X = \{x_n\}_{n=1}^N$, labels $Y = \{y_n\}_{n=1}^N$ (i.i.d)
- $x_n \in \mathcal{X}$ (we assume $\mathcal{X} = [0, 1]^D$ but could be more general)
- $y_n \in \{1, \ldots, K\}$ (classification) or $y_n \in \mathbb{R}$ (regression)
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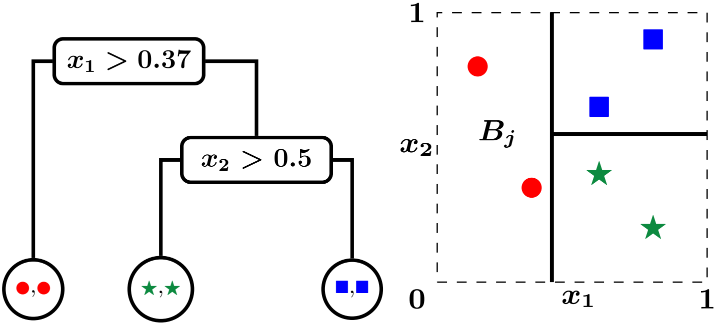
  - *Do we Need Hundreds of Classifiers to Solve Real World Classification Problems?* [Fernández-Delgado et al., 2014]
- What is a decision tree?

# Example: Classification tree

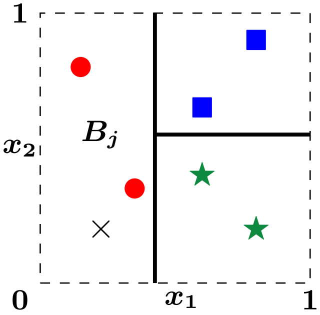
- Hierarchical axis-aligned binary partitioning of input space
- Rule for predicting label within each block




$\mathcal{T}$: list of nodes, feature-id + location of splits for internal nodes
$\boldsymbol{\theta}$: Multinomial parameters at leaf nodes

# Prediction using decision tree

- Example:
  - Multi-class classification: $\theta = [\theta_r, \theta_b, \theta_g]$
  - Prediction = smoothed empirical histogram in node $j$
  - Label counts in left node $[n_r = 2, n_b = 0, n_g = 0]$
  - $\theta \sim \mathcal{D}irichlet(\alpha/3, \alpha/3, \alpha/3)$
  - Prediction = Posterior mean of $\theta = \left[\frac{2+\alpha/3}{2+\alpha}, \frac{\alpha/3}{2+\alpha}, \frac{\alpha/3}{2+\alpha}\right]$



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  - Prediction = Posterior mean of $\theta = \left[\frac{2+\alpha/3}{2+\alpha}, \frac{\alpha/3}{2+\alpha}, \frac{\alpha/3}{2+\alpha}\right]$
- Likelihood for $n^{th}$ data point $= p(y_n|\theta_j)$ assuming $x_n$ lies in leaf node $j$ of $\mathcal{T}$
- Prior over $\theta_j$: independent or hierarchical
- Prediction for $x_*$ falling in $j = \mathbb{E}_{\theta_j|\mathcal{T},X,Y}\left[p(y_*|\theta_j)\right]$, where

$$p(\theta_j \mid \mathcal{T}, X, Y) \propto \underbrace{p(\theta_j|...)}_{\text{prior}} \underbrace{\prod_{n \in N(j)} p(y_n|\theta_j)}_{\text{likelihood of data points in node j}}$$

- Smoothing is done independently for each tree

# From decision trees to Random forests (RF)

- Generate randomized trees $\{\mathcal{T}_m\}_1^M$
- Prediction for $x_*$:

$$p(y_*|x_*) = \frac{1}{M}\sum_m p(y_*|x_*, \mathcal{T}_m)$$

- Model combination and not Bayesian model averaging

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- Advantages of RF
  - Excellent predictive performance (test accuracy)
  - Fast to train (in batch setting) and test
  - Trees can be trained in parallel

# Disadvantages of RF

- Not possible to train incrementally
  - Re-training batch version periodically is slow $\mathcal{O}(N^2 \log N)$
  - Existing online RF variants [Saffari et al., 2009, Denil et al., 2013] require
    - lots of memory / computation or
    - need lots of training data before they can deliver good test accuracy (data inefficient)

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    - lots of memory / computation or
    - need lots of training data before they can deliver good test accuracy (data inefficient)
- Random forests do not give useful uncertainty estimates
  - Predictions outside range of training data can be overconfident
  - Uncertainty estimates are crucial in applications such as Bayesian optimization, Just-in-time learning, reinforcement learning, etc.

# Mondrian Forests

**Mondrian forests** = Mondrian process + Random forests

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- Can operate in either batch mode or online mode
- Online speed $\mathcal{O}(N \log N)$
- Data efficient (predictive performance of online mode equals that of batch mode!)
- Better uncertainty estimate than random forests
- Predictions outside range of training data exhibit higher uncertainty and shrink to prior as you move farther away

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# Popular batch RF variants

How to generate individual trees in RF?

- **Breiman-RF** [Breiman, 2001]: Bagging + Randomly subsample features and choose best location amongst subsampled features

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How to generate individual trees in RF?

- **Breiman-RF** [Breiman, 2001]: Bagging + Randomly subsample features and choose best location amongst subsampled features
- **Extremely Randomized Trees** [Geurts et al., 2006] (ERT-$k$): Randomly sample $k$ (feature-id, location) pairs and choose the best split amongst this subset
  - no bagging
  - ERT-1 does not use labels $Y$ to guide splits!

# Mondrian process [Roy and Teh, 2009]

- MP($\lambda, \mathcal{X}$) specifies a distribution over hierarchical axis-aligned binary partitions of $\mathcal{X}$ (e.g. $\mathbb{R}^D$, $[0, 1]^D$)
- $\lambda$ is complexity parameter of the Mondrian process

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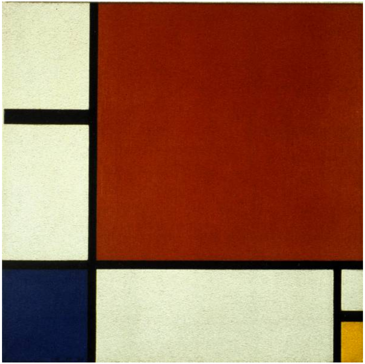
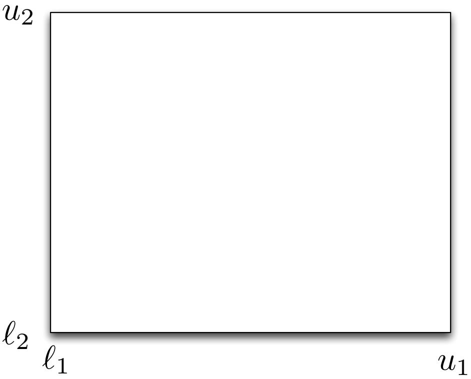


Figure: Mondrian Composition II in Red, Blue and Yellow (Source: Wikipedia)

# Generative process: MP$(\lambda, \{[\ell_1, u_1], [\ell_2, u_2]\})$

1. Draw $\Delta$ from exponential with rate $u_1 - \ell_1 + u_2 - \ell_2$
2. **IF** $\Delta > \lambda$ stop,



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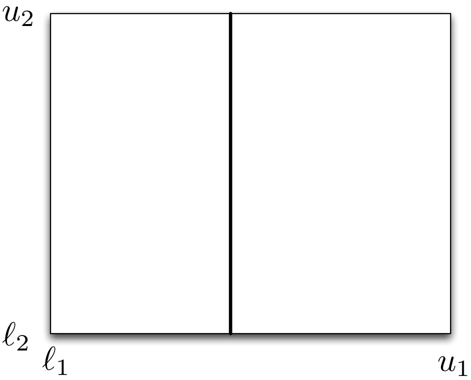
1. Draw $\Delta$ from exponential with rate $u_1 - \ell_1 + u_2 - \ell_2$
2. **IF** $\Delta > \lambda$ stop, **ELSE**, sample a split
   - split dimension: choose dimension $d$ with prob $\propto u_d - \ell_d$
   - split location: choose uniformly from $[\ell_d, u_d]$



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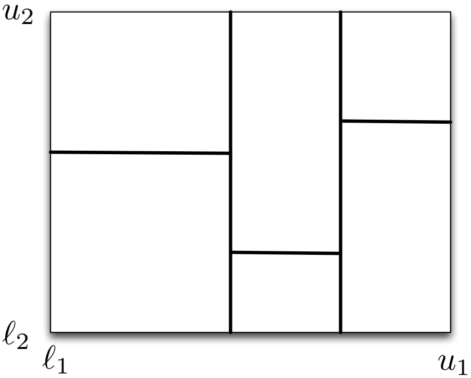
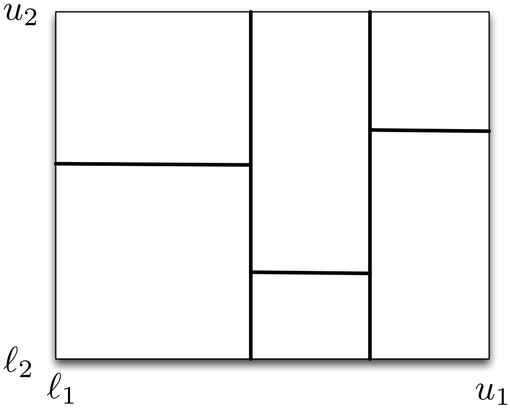
1. Draw $\Delta$ from exponential with rate $u_1 - \ell_1 + u_2 - \ell_2$
2. **IF** $\Delta > \lambda$ stop, **ELSE**, sample cut
   - Choose dimension $d$ with probability $\propto u_d - \ell_d$
   - Choose cut location uniformly from $[\ell_d, u_d]$
   - Recurse on left and right subtrees with parameter $\lambda - \Delta$



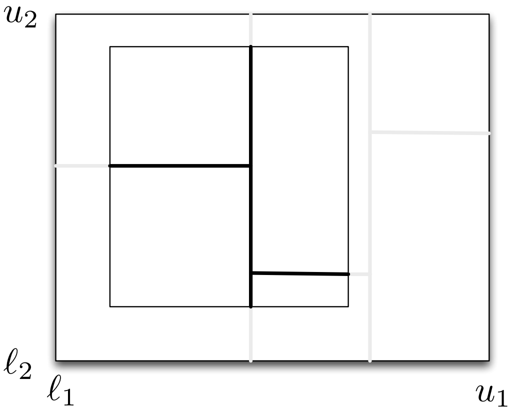
# Self-consistency of Mondrian process

- Simulate $\mathcal{T} \sim \mathrm{MP}(\lambda, [\ell_1, u_1], [\ell_2, u_2])$



# Self-consistency of Mondrian process

- Simulate $\mathcal{T} \sim \mathrm{MP}(\lambda, [\ell_1, u_1], [\ell_2, u_2])$
- Restrict $\mathcal{T}$ to a smaller rectangle $[\ell'_1, u'_1] \times [\ell'_2, u'_2]$



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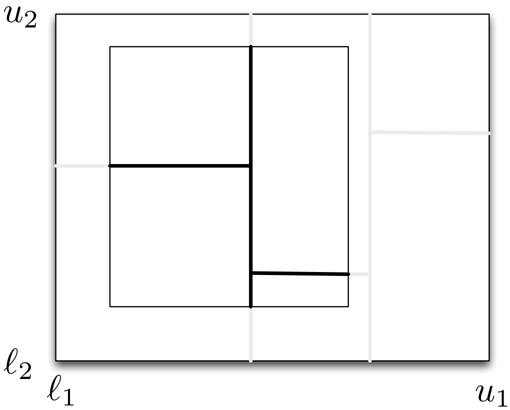


- Restriction has distribution $\mathrm{MP}(\lambda, [\ell'_1, u'_1], [\ell'_2, u'_2])$!

# Mondrian trees

- Use $X$ to define lower and upper limits within each node and use MP to sample splits.

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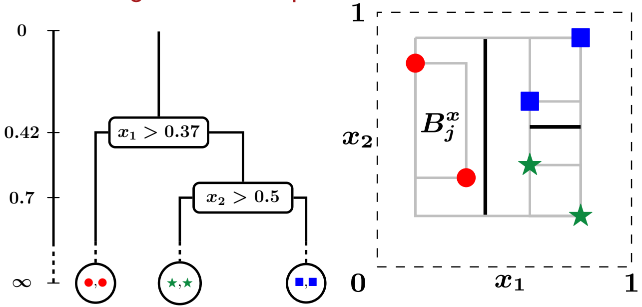
- Use $X$ to define lower and upper limits within each node and use MP to sample splits.
- Difference between Mondrian tree and usual decision tree
  - split in node $j$ is committed only within extent of training data in node $j$
  - node $j$ is associated with 'time of split' $t_j > 0$ (split time increases with depth and will be useful in online training)
  - splits are chosen independent of the labels Y
  - $\lambda$ is 'weighted max-depth'.



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# Mondrian trees: online learning

- As dataset grows, we extend the Mondrian tree $\mathcal{T}$ by simulating from a conditional Mondrian process MTx

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$$\begin{array}{c} \mathcal{T} \sim \mathrm{MT}(\lambda, \mathcal{D}_{1:n}) \\ \mathcal{T}' \mid \mathcal{T}, \mathcal{D}_{1:n+1} \sim \mathrm{MTx}(\lambda, \mathcal{T}, \mathcal{D}_{n+1}) \end{array} \implies \mathcal{T}' \sim \mathrm{MT}(\lambda, \mathcal{D}_{1:n+1})$$

- Distribution of batch and online trees are the same!
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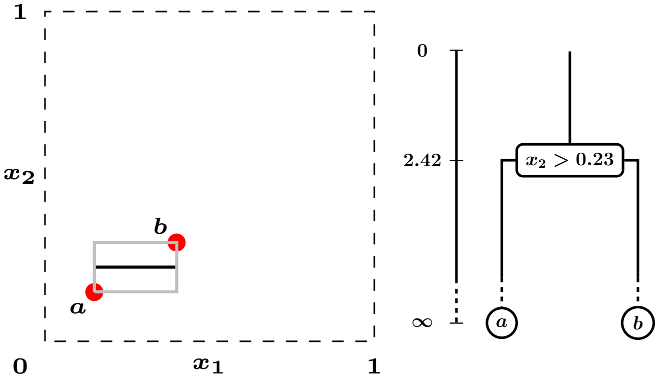
- Distribution of batch and online trees are the same!
- Order of the data points does not matter
- $\mathrm{MTx}$ can perform one or more of the following 3 operations
  - insert new split above an existing split
  - extend existing split to new range
  - split leaf further
- Computational complexity $\mathrm{MTx}$ is linear in depth of tree

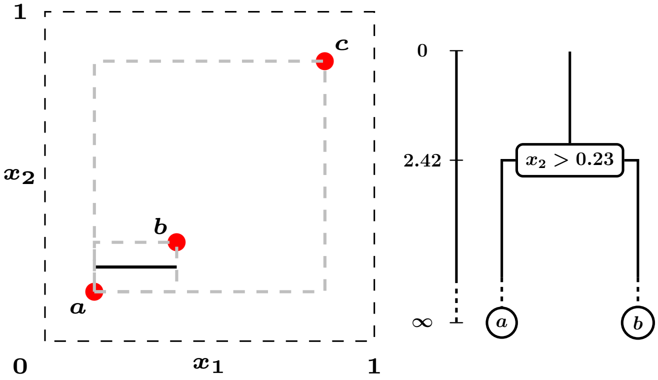
# Online training cartoon

Start with data points *a* and *b*



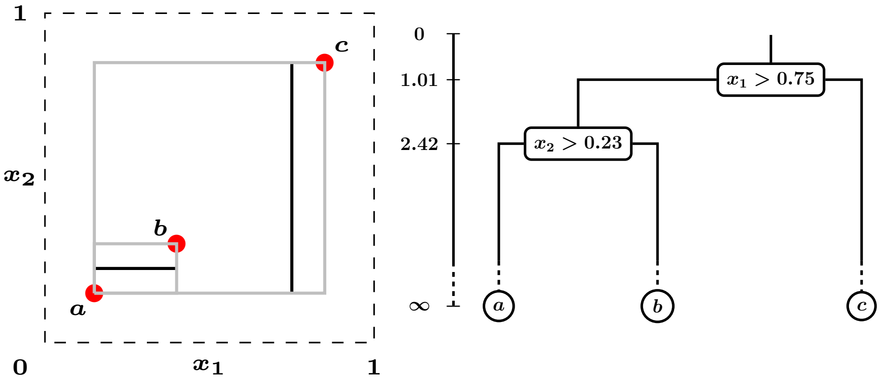
# Online training cartoon

Adding new data point $c$: update visible range



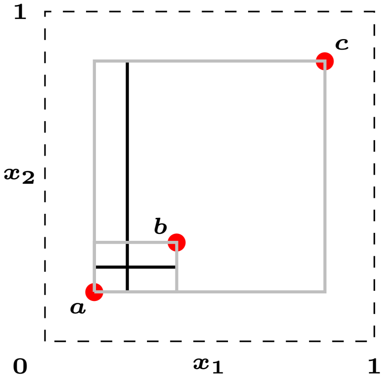
# Online training cartoon

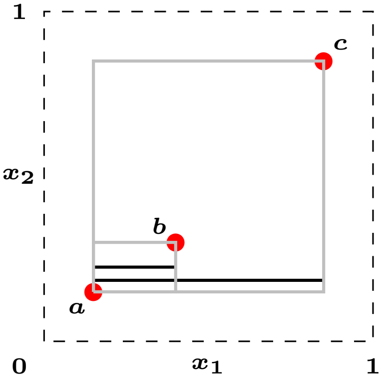
Adding new data point $c$: introduce new split (above an existing split). New split in $R_{abc}$ should be consistent with $R_{ab}$.



# Online training cartoon

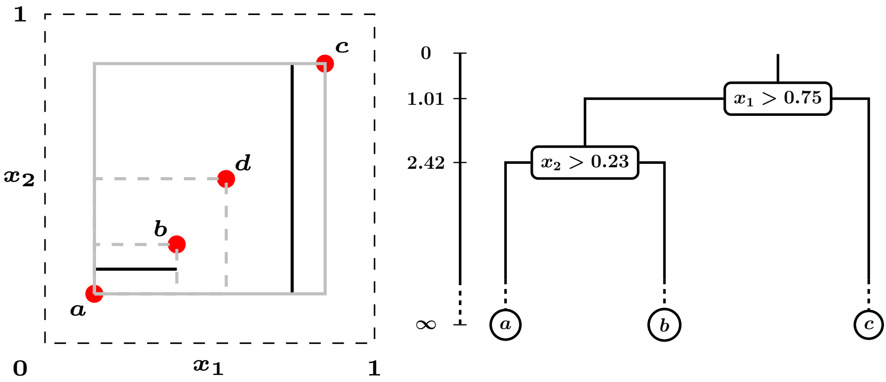
Examples of splits that are not self-consistent.



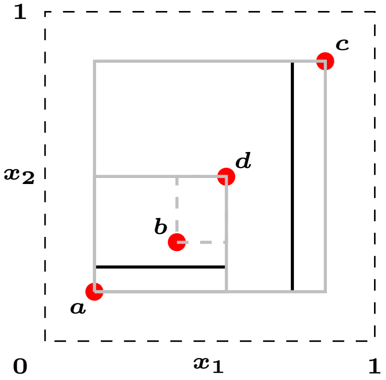
# Online training cartoon

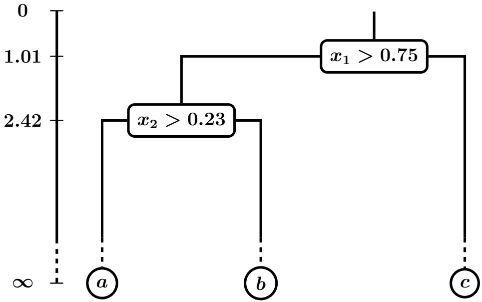
Adding new data point $d$: traverse to left child and update range



# Online training cartoon

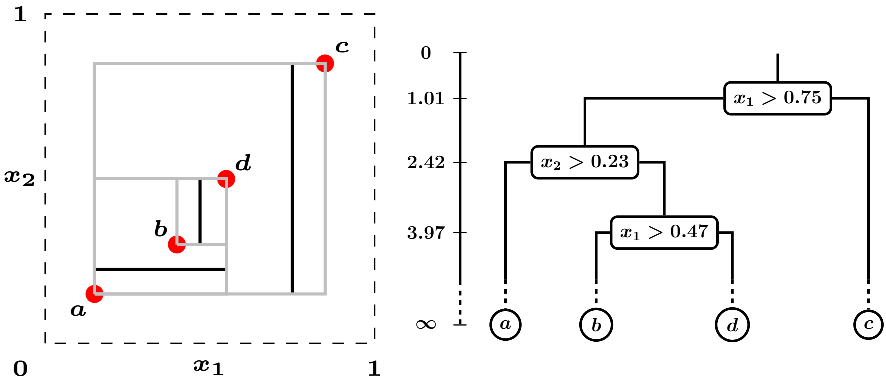
Adding new data point $d$: extend the existing split to new range



# Online training cartoon

Adding new data point *d*: split leaf further



# Key differences between Mondrian forests and existing online random forests

- Splits extended in a self-consistent fashion
- Splits not extended to unobserved regions
- New split can be introduced *anywhere* in the tree (as long as it's consistent with subtree below)

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# Prediction and Hierarchical smoothing

- Extend Mondrian to range of test data
  - Test data point can potentially branch off and form separate leaf node of its own!
  - Points far away from range of training data are more likely to brach off
  - We analytically average over every possible extension

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  - Test data point can potentially branch off and form separate leaf node of its own!
  - Points far away from range of training data are more likely to brach off
  - We analytically average over every possible extension
- Hierarchical smoothing for posterior mean of $\theta|\mathcal{T}$
  - Independent prior would predict from prior if test data branches off into its own leaf node
  - Bayesian smoothing done independently within each tree
  - Ensemble: model combination and not BMA

# Prediction and Hierarchical smoothing

- Classification
  - Multinomial likelihoods, Hierarchical Normalized Stable process prior [Wood et al., 2009]
  - Fast approximate inference using Interpolated Kneser Ney approximation
- Regression
  - Gaussian likelihood, Gaussian prior
  - Fast exact inference using belief propagation
- Both models are closed under marginalization, so introducing new nodes does not change the model

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# Classification: Experimental setup

- Competitors
  - Periodically re-trained batch versions (RF, ERT)
  - Online RF [Saffari et al., 2009]

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- Competitors
  - Periodically re-trained batch versions (RF, ERT)
  - Online RF [Saffari et al., 2009]
- Datasets:

| Name | $D$ | #Classes | #Train | #Test |
|---|---|---|---|---|
| *Satellite images* | 36 | 6 | 3104 | 2000 |
| *Letter* | 16 | 26 | 15000 | 5000 |
| *USPS* | 256 | 10 | 7291 | 2007 |
| *DNA* | 180 | 3 | 1400 | 1186 |

- Training data split into 100 mini batches (unfair to MF)
- Number of trees $= 100$

# Classification results: Letter dataset

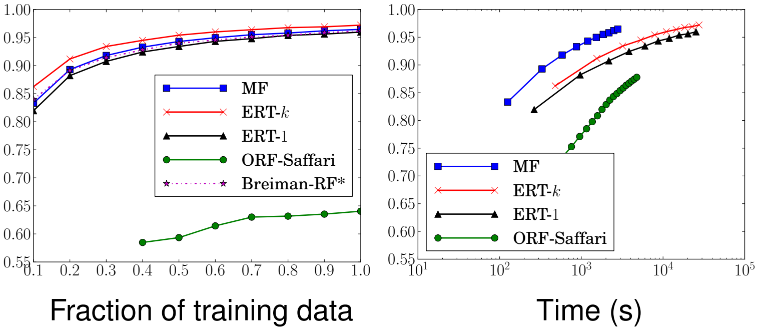



Figure: Test accuracy

- Data efficiency: Online MF very close to batch RF (ERT, Breiman-RF) and significantly outperforms ORF-Saffari
- Speed: MF much faster than periodically re-trained batch RF and ORF-Saffari

# Classification results: USPS dataset

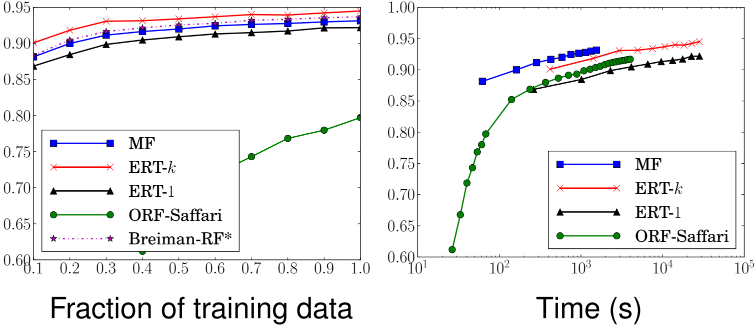



Figure: Test accuracy

# Classification results: Satellite Images dataset

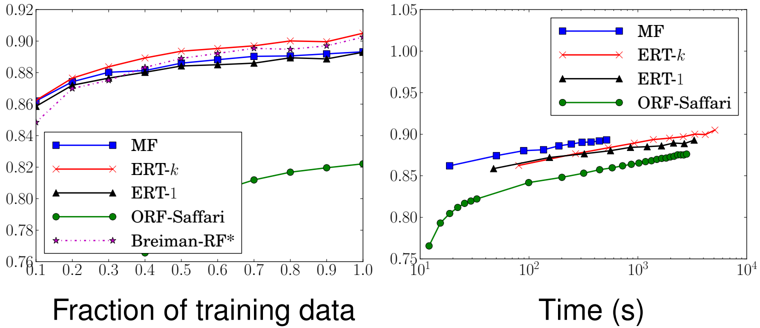



Figure: Test accuracy

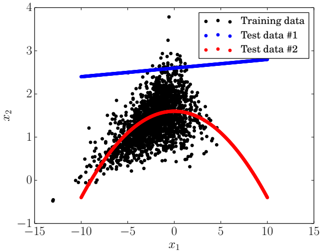
# Outline

# Uncertainty estimation: Experimental setup

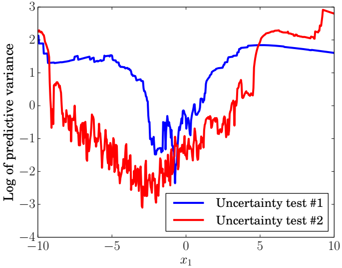
- Application: Just-In-Time learning in Expectation Propagation [Jitkrittum et al., 2015]
- Goal: learn to predict output message from incoming messages
  - If current input is similar to previous input, use estimate
  - Whenever estimate is uncertain, evaluate the true value

# Uncertainty estimation: Experimental setup

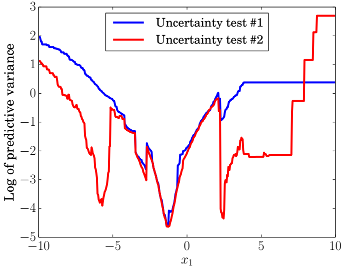
- Application: Just-In-Time learning in Expectation Propagation [Jitkrittum et al., 2015]
- Goal: learn to predict output message from incoming messages
  - If current input is similar to previous input, use estimate
  - Whenever estimate is uncertain, evaluate the true value
- Setup: Test dataset differs from training dataset
- Desiderata: Predictions should exhibit higher uncertainty as we move farther away
- How does MF uncertainty compare to other RFs?



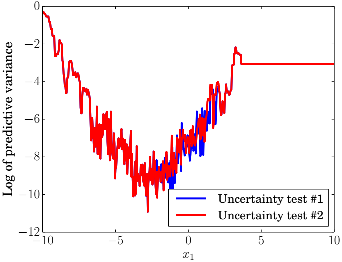

(a) Distribution of train/test inputs (labels not depicted)




(b) Uncertainty estimate of MF




(c) Uncertainty estimate of ERT




(d) Uncertainty of Breiman-RF

# Comparison to large-scale Gaussian processes

- Experiments on airline delay dataset [Hensman et al., 2013]
- Large scale approximate Gaussian processes:
  - Variational approximations: SVI-GP [Hensman et al., 2013] and Dist-VGP [Gal et al., 2014]
  - Combine GP outputs from subsets of data: robust BCM (rBCM) [Deisenroth and Ng, 2015]

| | 700K/100K RMSE | NLPD | 2M/100K RMSE | NLPD | 5M/100K RMSE | NLPD |
|---|---|---|---|---|---|---|
| SVI-GP | 33.0 | - | - | - | - | - |
| Dist-VGP | 33.0 | - | - | - | - | - |
| rBCM | 27.1 | 9.1 | 34.4 | 8.4 | **35.5** | 8.8 |
| Breiman-RF | **24.07** $\pm$ **0.02** | | **27.3** $\pm$ **0.01** | | 39.47 $\pm$ 0.02 | |
| ERT | 24.32 $\pm$ 0.02 | | 27.95 $\pm$ 0.02 | | 38.38 $\pm$ 0.02 | |
| MF | 26.57 $\pm$ 0.04 | **4.89** $\pm$ **0.02** | 29.46 $\pm$ 0.02 | **4.97** $\pm$ **0.01** | 40.13 $\pm$ 0.05 | **6.91** $\pm$ **0.06** |

So, what’s the catch?

# DNA (classification with irrelevant features)

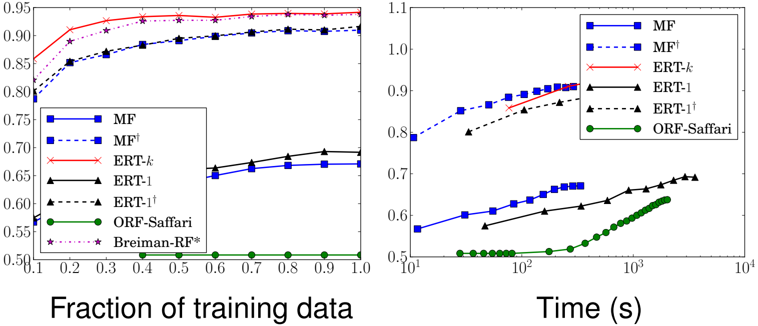



Figure: Test accuracy

- Irrelevant features: Choosing splits independent of labels (MF, ERT-1) harmful in presence of irrelevant features
- Removing irrelevant features (use only the 60 most relevant features[1]) improves test accuracy (MF$^{\dagger}$, ERT-1$^{\dagger}$)

[1] https://www.sgi.com/tech/mlc/db/DNA.names

# Conclusion

- Mondrian Forests (attempt to) combine the strengths of random forests and Bayesian non-parametrics
  - Computationally faster compared to existing online RF and periodically re-trained batch RF
  - Data efficient compared to existing online RF
  - Better uncertainty estimates than existing random forests

# Conclusion

- Mondrian Forests (attempt to) combine the strengths of random forests and Bayesian non-parametrics
  - Computationally faster compared to existing online RF and periodically re-trained batch RF
  - Data efficient compared to existing online RF
  - Better uncertainty estimates than existing random forests
- Future work
  - Mondrian forests for high dimensional data with lots of irrelevant features
  - Explore other likelihoods and hierarchical models (e.g. linear regression at leaf node will extrapolate better)

- *Mondrian Forests: Efficient Online Random Forests, NIPS 2014*
- *Mondrian Forests for Large-Scale Regression when Uncertainty Matters, arXiv:1506.03805, 2015*

http://www.gatsby.ucl.ac.uk/~balaji

Thank you!

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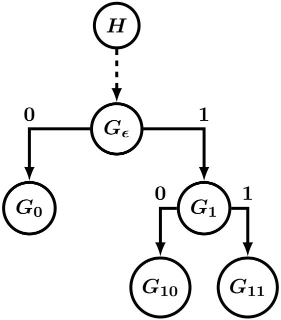
Extra slides

# Hierarchical prior over $\theta$




- $G_j$ parametrizes $p(y|x)$ in $B_j^x$
- Normalized stable process (NSP): special case of PYP where concentration = 0
- $d_j \in (0, 1)$ is discount for node $j$
- $G_\epsilon | H \sim \text{NSP}(d_\epsilon, H)$,
  $G_{j0} | G_j \sim \text{NSP}(d_{j0}, G_j)$,
  $G_{j1} | G_j \sim \text{NSP}(d_{j1}, G_j)$
- $\mathbb{E}[G_\epsilon(s)] = H(s)$
- $\mathrm{Var}[G_\epsilon(s)] = (1 - d_H) H(s) \big(1 - H(s)\big)$
- Closed under Marginalization: $G_0 | H \sim \text{NSP}(d_\epsilon d_0, H)$
- $d_j = e^{-\gamma \Delta_j}$ where $\Delta_j = t_j - t_{\text{parent}(j)}$ (time difference between split times)

# Posterior inference for NSP

- Special case of approximate inference for PYP [Teh, 2006]
- Chinese restaurant process representation
- **Interpolated Kneser-Ney smoothing**
  - fast approximation
  - Restrict number of tables serving a dish to at most 1
  - popular smoothing technique in language modeling

# Interpolated Kneser-Ney smoothing

- Prediction for $x_*$ lying in node $j$ is given by

$$\overline{G}_{jk} = p(y_* = k | x_* \in B_j^x, X, Y, \mathcal{T})$$
$$= \begin{cases} \dfrac{c_{j,k} - d_j \, \text{tab}_{j,k}}{c_{j,\cdot}} + \dfrac{d_j \, \text{tab}_{j,\cdot}}{c_{j,\cdot}} \, \overline{G}_{\text{parent}(j),k} & c_{j,\cdot} > 0 \\ \overline{G}_{\text{parent}(j),k} & c_{j,\cdot} = 0 \end{cases}$$

- $c_{j,k}$ = number of points in node $j$ with label $k$
- $\text{tab}_{j,k} = \min(c_{j,k}, 1)$ and $d_j = \exp\big(-\gamma(t_j - t_{\text{parent}(j)})\big)$