Avoiding Bias from Feature Selection

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Outline of the talk

- Introduction to Classification Problems
- Challenge from High Dimensional Features
- Bias from Feature Selection
- A Method for Avoiding Bias from Feature Selection
- Application to Naive Bayes Classification Model
  - Definition of Naive Bayes Classification Model
  - Predictions for Test Cases
  - Computation of Adjustment Factor
  - Demonstration with Simulated and Real Datasets
- Conclusion and Discussion

Introduction to Classification Problems

- Goal: Given a feature vector x, we want to predict the associated response y, i.e. find a predictive function C from x to y:

$$y = C(x)$$

- Probabilistic Classification: A better way is to report the predictive distribution of y given x:

$$P(y \mid x)$$

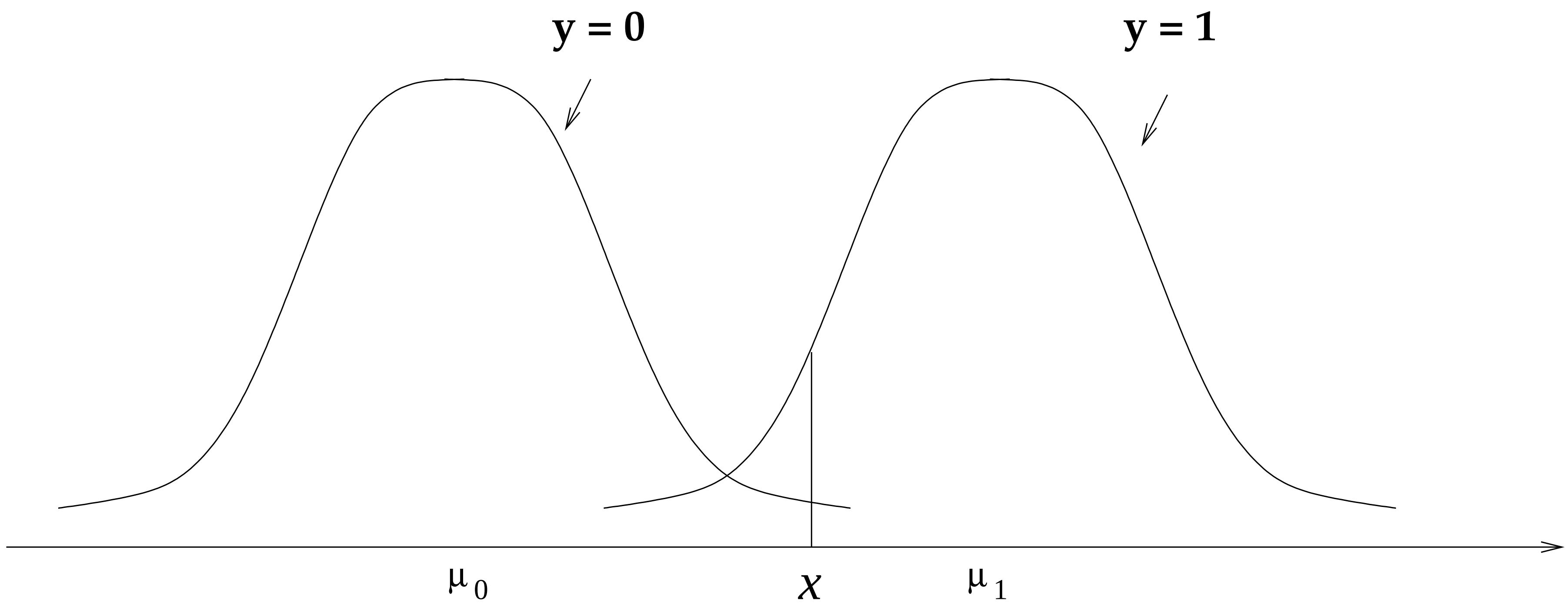
- Statistical Method: Estimate $P(y \mid x)$ by learning from the available data $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$, collectively $\{x^{\text{train}}, y^{\text{train}}\}$, called training data
- Examples:
  - Given the image of handwritten digit, recognize the digit on it
  - Given the content of a message, determine whether it is a spam
  - Given gene expression data of a patient, classify the type of tumor

Model-based Classification

Model $P(y)$ and $P(x \mid y)$, or model $P(y, x)$ directly, then $P(y \mid x)$ is found by Bayes rule:

$$P(y \mid x) = P(y, x)/P(x) = P(y)\, P(x \mid y)/P(x)$$

Illustration with a simple example:



Bayesian Statistical Classification

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- Updating our knowledge for θ in light of training data $x^{\text{train}}, y^{\text{train}}$:

  $$P(\theta \mid x^{\text{train}}, y^{\text{train}}) = \frac{P(x^{\text{train}}, y^{\text{train}} \mid \theta) \ P(\theta)}{P(x^{\text{train}}, y^{\text{train}})}$$

  This is called posterior distribution of θ given $x^{\text{train}}, y^{\text{train}}$.

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- The joint distribution of x^*, y^* for a test case is found with updated information of θ:

$$P(x^*, y^* \mid x^{\text{train}}, y^{\text{train}}) = \int P(x^*, y^* \mid x^{\text{train}}, y^{\text{train}}, \theta) \ P(\theta \mid x^{\text{train}}, y^{\text{train}}) \ d\theta$$

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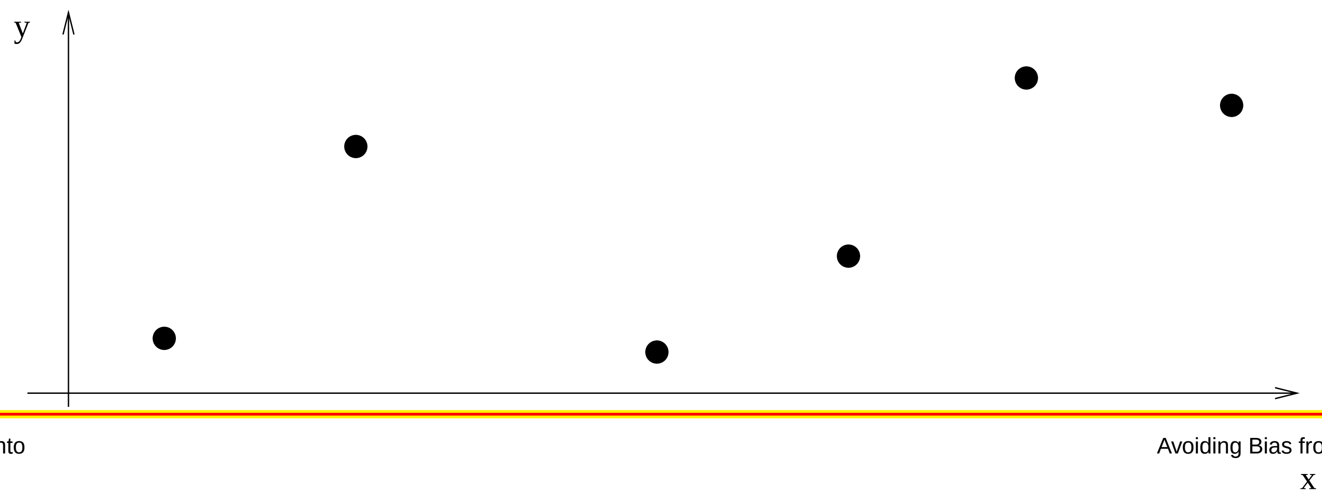

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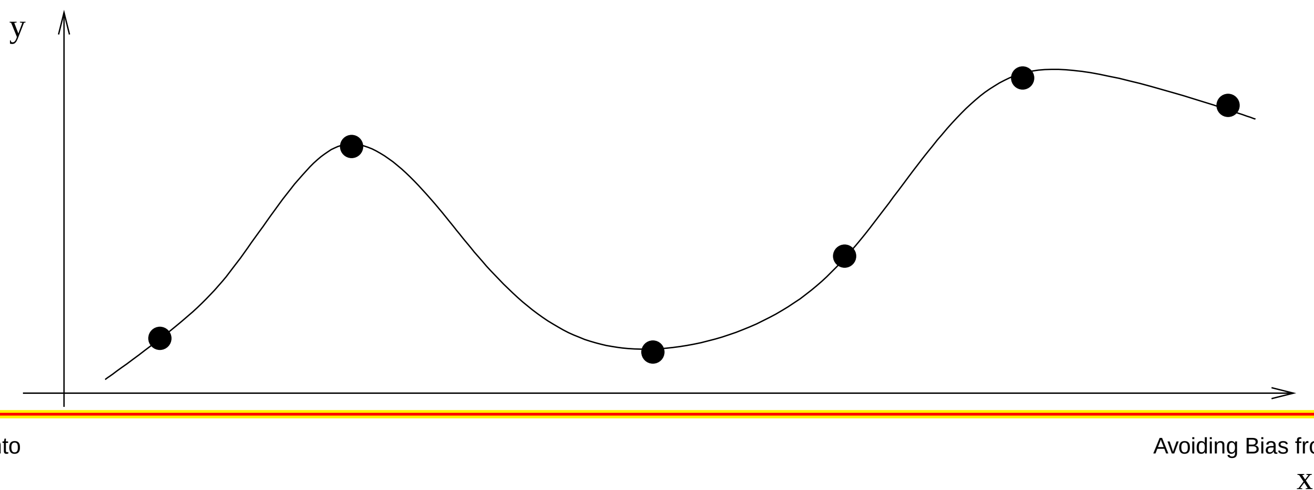

Bias from Feature Selection

For previous reasons, one may like to select a subset of features to use based on some measure of the dependency, such as absolute correlation, with y. However, this procedure will introduce an optimistic bias, i.e., the relationship between y and x appears stronger than it actually is, which can be phrased in following ways:

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- Underestimation of prediction errors: e.g.
  If y^* is binary, and guess y^* by thresholding the predictive probability $\hat{p}^*$ at $1/2$, the *expected (estimated) error rate*, defined as

  $$\hat{p}^* \, I(\hat{p}^* < 1/2) + (1 - \hat{p}^*) \, I(\hat{p}^* \geq 1/2),$$

  is smaller than the actual error rate.

A Method for Avoiding Bias from Features Selection

- Idea: Our predictions should condition not only on the retained features $x_{1:k}^{\text{train}}$, but also on the fact that the other $p-k$ features have sample correlation with the response that is less than γ in absolute value:

$$y^{\text{train}}, \quad x_{1:k}^{\text{train}}, \quad |\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \le \gamma \text{ for } t = k+1, \ldots, p$$

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- Models: The response and the predictors are modeled jointly. Given the response y and a model parameter α, the features $x_1, \ldots, x_p$, are modeled to be independent and has identical distribution:

$$P(x_1, \cdots, x_p \mid y, \alpha) = \prod_{t=1}^{p} \Big[P(x_t \mid y, \alpha) \Big]$$

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- Adjustment factor: The likelihood function of α based on $y^{\text{train}}, x_{1:k}^{\text{train}}$ is multiplied by:

$$\begin{aligned} & P(\, |\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \leq \gamma \text{ for } t = k+1, \ldots, p \mid \alpha, y^{\text{train}}) \\ = \quad & \Big[P(\, |\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \leq \gamma \mid \alpha, y^{\text{train}}) \Big]^{p-k} \end{aligned}$$

Remark: we need to compute the adjustment factor only once regardless how many features are discarded.

Bayesian Naive Bayes Model for Binary Data

Data distribution:

$$
\begin{aligned}
y^{(i)} \mid \psi &\sim \text{Bernoulli}\,(\psi), \quad \text{for } i = 1, \ldots, n \\
x_j^{(i)} \mid y^{(i)}, \boldsymbol{\phi} &\sim \text{Bernoulli}\,(\phi_{y^{(i)},j}) \quad \text{for } i = 1, \ldots, n \text{ and } j = 1, \ldots, p
\end{aligned}
$$

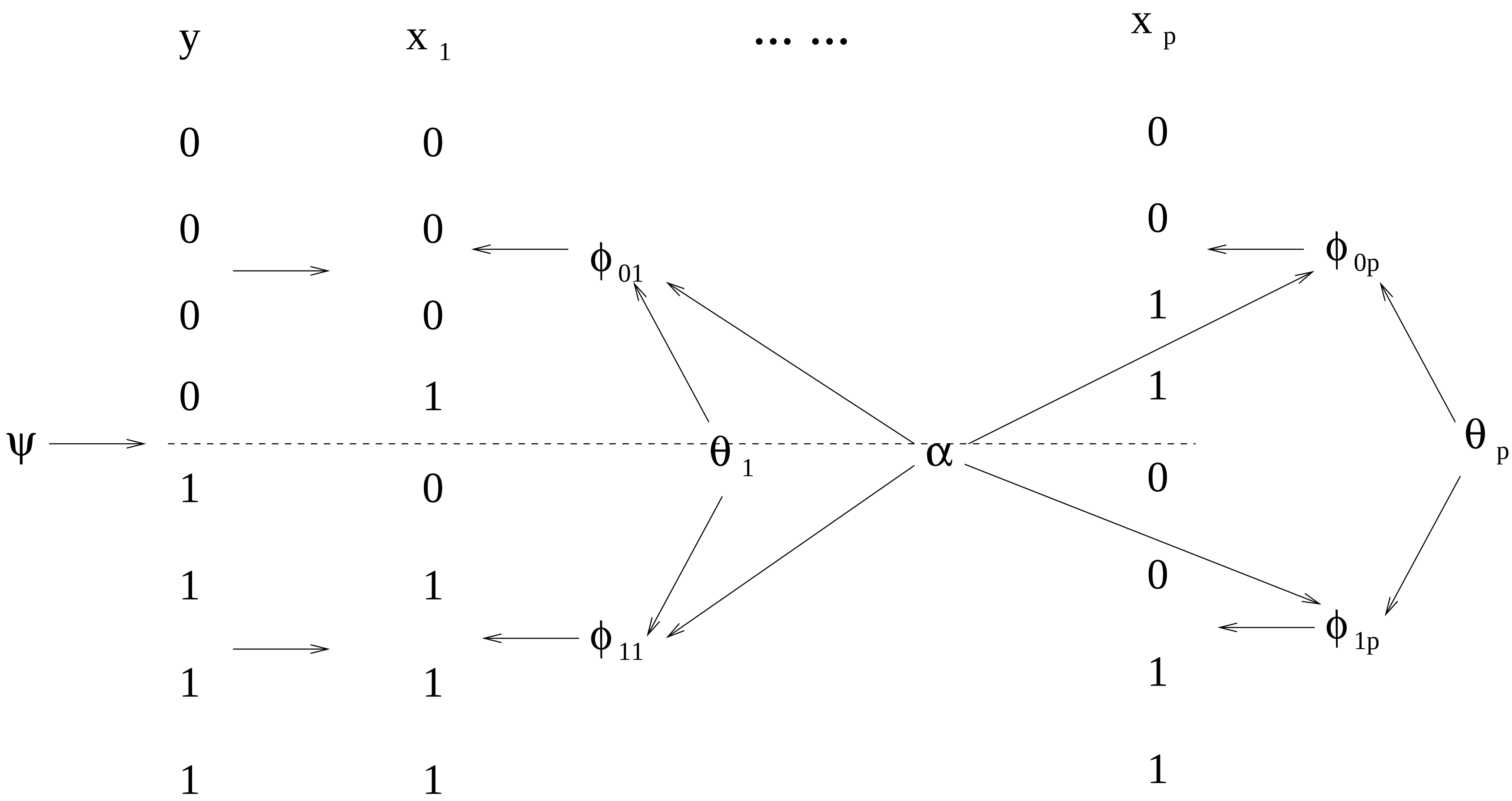
Prior distribution:

$$
\begin{aligned}
\psi &\sim \text{Beta}\,(f_1, f_0) \\
\phi_{0,j},\, \phi_{1,j} \mid \alpha,\, \theta_j &\overset{\text{IID}}{\sim} \text{Beta}\,(\alpha\theta_j,\, \alpha(1-\theta_j)), \quad \text{for } j = 1, \ldots, p \\
\alpha &\sim \text{Inverse-Gamma}(a, b) \\
\theta_1, \ldots, \theta_p &\overset{\text{IID}}{\sim} \text{Uniform}(0, 1)
\end{aligned}
$$

Note:

$$
\begin{aligned}
\text{E}(\phi_{yj}) &= \theta_j \\
\text{Var}(\phi_{yj}) &= \theta_j(1-\theta_j)/(\alpha+1)
\end{aligned}
$$

A Picture of Bayesian Naive Bayes Model



Obtaining $P(y^* \mid y^{\text{train}})$

For the model defined previously, $P(y^* \mid y^{\text{train}})$, which is needed to find the conditional $P(y^* \mid x^*, x^{\text{train}}, y^{\text{train}})$, is found to be:

$$P(y^* \mid y^{\text{train}}) \quad = \quad \text{Bernoulli}\,(y^*; \hat{\psi})$$

where $\hat{\psi} = (f_1 + N_1) \,/\, (f_0 + f_1 + n)$.

$$\begin{array}{lll} & f_1 \searrow & \\ y^{\text{train}}\ : & & \psi \longrightarrow \underbrace{0 \quad 0 \quad 0 \quad 0}_{n - N_1} \quad \underbrace{1 \quad 1 \quad 1 \quad 1}_{N_1} \\ & f_0 \nearrow & \end{array}$$

In more details, $P(y^{\text{train}})$ is computed as follows:

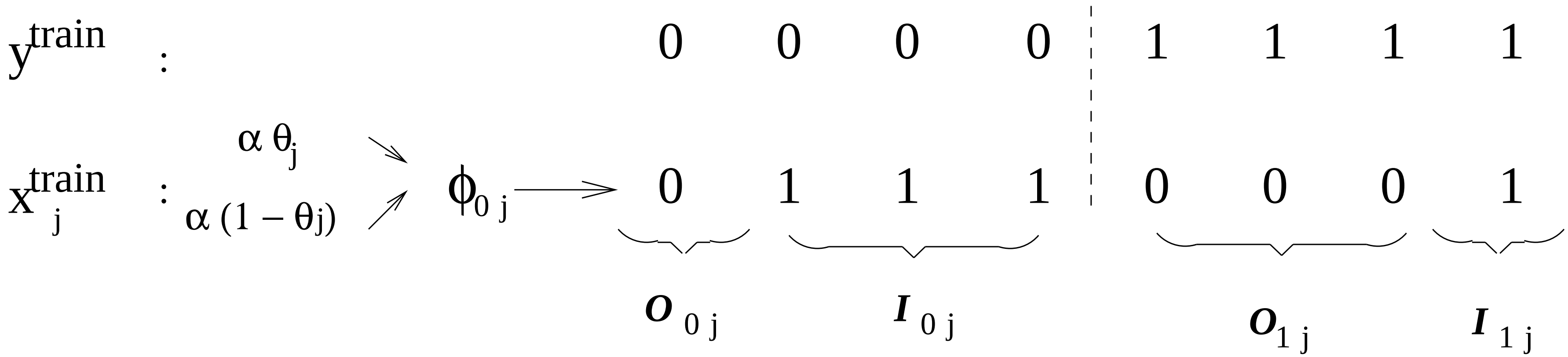
$$\begin{aligned} P(y^{\text{train}}) &= \int_0^1 \frac{\Gamma(f_0+f_1)}{\Gamma(f_0)\Gamma(f_1)} \psi^{f_1} (1 - \psi)^{f_0}\ \psi^{\sum\limits_{i=1}^{n} I(y^{(i)}=1)}\ (1-\psi)^{\sum\limits_{i=1}^{n} I(y^{(i)}=0)} d\psi \\ &= U\Big(f_0,\ f_1,\ \sum_{i=1}^{n}\ I\big(y^{(i)}=0\big),\ \sum_{i=1}^{n}\ I\big(y^{(i)}=1\big)\Big) \end{aligned}$$

Obtaining $P(x_j^* \mid \theta_j,\, \alpha,\, x_j^{\text{train}},\, y^{\text{train}},\, y^*)$

Similarly,

$$P(x_j^* \mid \theta_j,\, \alpha,\, x_j^{\text{train}},\, y^{\text{train}},\, y^*) = \text{Bernoulli}\,(x_j^*; \hat{\phi}_{y^*,j})$$

where $\hat{\phi}_{y^*,j} = (\alpha\theta_j + I_{y^*,j}) \,/\, (\alpha + N_{y^*})$ and $I_{y,j} \;=\; \sum_{i=1}^{n} I(y^{(i)} = y,\, x_j^{(i)} = 1)$.



Predictions for test cases (I)

- Using only retained features:

$$P(y^* \mid x^*_{1:k},\, x^{\text{train}}_{1:k},\, y^{\text{train}}) \quad = \quad \frac{P(y^* \mid y^{\text{train}})\, P(x^*_{1:k} \mid y^*,\, x^{\text{train}}_{1:k},\, y^{\text{train}})}{\displaystyle\sum_{y=0}^{1} P(y^* = y \mid y^{\text{train}})\, P(x^*_{1:k} \mid y^* = y,\, x^{\text{train}}_{1:k},\, y^{\text{train}})}$$

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$$P(x^*_{1:k} \mid y^*,\, x^{\text{train}}_{1:k},\, y^{\text{train}}) \;=\; \frac{P(x^*_{1:k},\, x^{\text{train}}_{1:k} \mid y^*,\, y^{\text{train}})}{P(x^{\text{train}}_{1:k} \mid y^{\text{train}})} \;\propto\; P(x^*_{1:k},\, x^{\text{train}}_{1:k} \mid y^*,\, y^{\text{train}})$$

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$$\begin{aligned} P(x^*_{1:k},\, x^{\text{train}}_{1:k} \mid y^*,\, y^{\text{train}}) &= \int P(\alpha)\, P(x^*_{1:k},\, x^{\text{train}}_{1:k} \mid \alpha,\, y^*,\, y^{\text{train}})\, d\alpha \\ &= \int P(\alpha) \prod_{j=1}^{k} P(x^*_j,\, x^{\text{train}}_j \mid \alpha,\, y^*,\, y^{\text{train}})\, d\alpha \end{aligned}$$

The above integral about α is approximated with Midpoint Rule.

Predictions for test cases (II)

$$
\begin{aligned}
& P(x_j^*,\, x_j^{\text{train}} \mid \alpha,\, y^*,\, y^{\text{train}}) \\
&= \int_0^1 P(x_j^* \mid \theta_j,\, \alpha,\, x_j^{\text{train}},\, y^{\text{train}},\, y^*)\, P(x_j^{\text{train}} \mid \theta_j,\, \alpha,\, y^{\text{train}})\, d\theta_j \\
&= \int_0^1 \text{Bernoulli}\,(x_j^*; \hat{\phi}_{y^*,j}) \prod_{y=0}^{1} U(\alpha\theta_j,\, \alpha(1-\theta_j),\, I_{y,j},\, O_{y,j})\, d\theta_j
\end{aligned}
$$

The above integral about θ_j is approximated with Simpson's Rule.

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- With correction for feature selection

$P(x_{1:k}^*,\, x_{1:k}^{\text{train}},\, \mid y^*,\, y^{\text{train}})$ is replaced with $P(x_{1:k}^*,\, x_{1:k}^{\text{train}}, \mathcal{S} \mid y^*,\, y^{\text{train}})$:

$$
P(x_{1:k}^*,\, x_{1:k}^{\text{train}},\, \mathcal{S} \mid y^*,\, y^{\text{train}}) = \int P(\alpha) P(\mathcal{S} \mid \alpha, y^{\text{train}}) \prod_{j=1}^{k} P(x_j^*, x_j^{\text{train}} \mid \alpha, y^*, y^{\text{train}}) d\alpha
$$

where $P(\mathcal{S} \mid \alpha,\, y^{\text{train}}) = \Big[P(|\text{COR}(y^{\text{train}}, x_t^{\text{train}})| \le \gamma \mid \alpha,\, y^{\text{train}}) \Big]^{p-k}$

Computation of the adjustment factor (I)

$\text{COR}(x_t^{\text{train}}, y^{\text{train}})$ can be written in terms of $I_0 = \sum_{i=1}^n I(y^{(i)} = 0,\, x_t^{(i)} = 1)$ and $I_1 = \sum_{i=1}^n I(y^{(i)} = 1,\, x_t^{(i)} = 1)$:

$$
\begin{aligned}
\text{COR}(x_t^{\text{train}},\, y^{\text{train}}) &= \frac{\displaystyle\sum_{i=1}^{n} \left(y^{(i)} - \bar{y}\right) x_t^{(i)}}{\sqrt{\displaystyle\sum_{i=1}^{n} \left(y^{(i)} - \bar{y}\right)^2} \sqrt{\displaystyle\sum_{i=1}^{n} \left(x_t^{(i)} - \bar{x}_t\right)^2}} \\
&= \frac{(0 - \overline{y})\, I_0 \;+\; (1 - \overline{y})\, I_1}{\sqrt{n\overline{y}(1-\overline{y})}\, \sqrt{I_0 + I_1 - (I_0 + I_1)^2/n}}
\end{aligned}
$$

I_0,I_1 are visualized:

$$
\begin{array}{ll}
y^{\text{train}} : & 0 \quad 0 \quad 0 \quad 0 \;\vdots\; 1 \quad 1 \quad 1 \quad 1 \\[1em]
x_t^{\text{train}} : & \underbrace{0}_{\boldsymbol{O}_0} \quad \underbrace{1 \quad 1 \quad 1}_{\boldsymbol{I}_0} \;\vdots\; \underbrace{0 \quad 0 \quad 0}_{\boldsymbol{O}_1} \quad \underbrace{1}_{\boldsymbol{I}_1}
\end{array}
$$

Computation of the adjustment factor (II)

An example showing values of $|\text{COR}(x_t^{\text{train}}, y^{\text{train}})|$ in terms of I_0 and I_1:

I_1 \ I_0	0	1	2	3	4	5	6	7	8
14	+1.00	+0.90	+0.81	+0.72	+0.62	+0.53	+0.42	+0.29	0.00
13	+0.91	+0.80	+0.70	+0.60	+0.49	+0.38	+0.25	+0.09	−0.16
12	+0.83	+0.72	+0.61	+0.50	+0.39	+0.27	+0.13	−0.03	−0.24
11	+0.76	+0.64	+0.52	+0.41	+0.30	+0.17	+0.04	−0.11	−0.30
10	+0.69	+0.57	+0.45	+0.33	+0.21	+0.09	−0.04	−0.18	−0.36
9	+0.63	+0.50	+0.38	+0.26	+0.14	+0.02	−0.11	−0.25	−0.41
8	+0.57	+0.44	+0.31	+0.19	+0.07	−0.05	−0.18	−0.31	−0.46
7	+0.52	+0.38	+0.24	+0.12	0.00	−0.12	−0.24	−0.37	−0.52
6	+0.46	+0.31	+0.18	+0.05	−0.07	−0.19	−0.31	−0.44	−0.57
5	+0.41	+0.25	+0.11	−0.02	−0.14	−0.26	−0.38	−0.50	−0.63
4	+0.36	+0.18	+0.04	−0.09	−0.21	−0.33	−0.45	−0.57	−0.69
3	+0.30	+0.11	−0.04	−0.17	−0.30	−0.41	−0.52	−0.64	−0.76
2	+0.24	+0.03	−0.13	−0.27	−0.39	−0.50	−0.61	−0.72	−0.83
1	+0.16	−0.09	−0.25	−0.38	−0.49	−0.60	−0.70	−0.80	−0.91
0	0.00	−0.29	−0.42	−0.53	−0.62	−0.72	−0.81	−0.90	−1.00

Computation of the adjustment factor (III)

- $P(I_0,\, I_1 \mid \alpha,\, y^{\text{train}})$ is symmetric for H_+ and H_-, so

$$P(\,|\text{COR}(x_t^{\text{train}}, y^{\text{train}})| \le \gamma \mid \alpha,\, y^{\text{train}}) \;=\; 1 - 2 \sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, y^{\text{train}})$$

- Conditioning on θ_t:

$$\sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, y^{\text{train}}) \;=\; \int_0^1 \sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}})\, d\theta_t$$

The above integration about θ_t is approximated with Simpson's Rule.

- $|\text{COR}(x_t^{\text{train}}, y^{\text{train}})|$ is monotone with respect to I_0 or I_1, so

$$\sum_{(I_0,I_1)\,\in\, H_+} P(I_0,\, I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \;=\; \sum_{I_1=b_0}^{n\overline{y}} \sum_{I_0=0}^{r_{I_1}} P(I_0,\, I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}})$$

- I_0 and I_1 are independent given $\alpha,\, \theta_t,\, y^{\text{train}}$, so

$$P(I_0,\, I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \;=\; P(I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) P(I_0 \mid \alpha,\, \theta_t,\, y^{\text{train}})$$

Computation of the adjustment factor (IV)

Finally, we can easily compute probability of I_0 and I_1:

$$P(I_1 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \;=\; \binom{N_1}{I_1} U(\alpha\theta_t,\, \alpha(1-\theta_t),\, I_1,\, N_1 - I_1)$$

and

$$P(I_0 \mid \alpha,\, \theta_t,\, y^{\text{train}}) \;=\; \binom{n - N_1}{I_0} U(\alpha\theta_t,\, \alpha(1-\theta_t),\, I_0,\, n - N_1 - I_0)$$

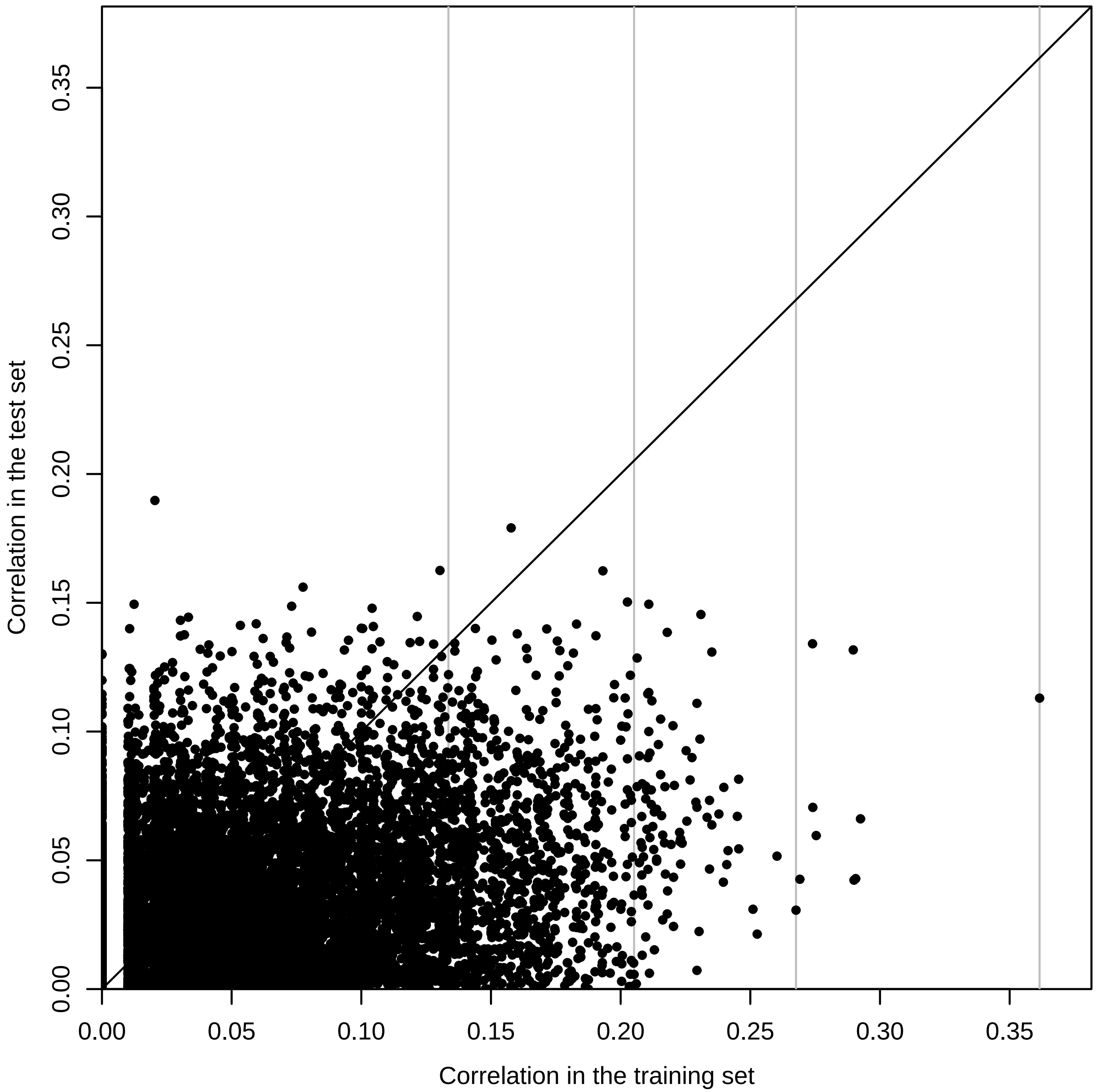
A Simulation Experiment

- Generating data: $\alpha = 300$, $p = 10000$, 100 training cases, 2000 test cases

- Selecting features: 4 subsets with only 1, 10, 100 and 1000 features were selected, with smallest absolute value of correlation being 0.36,0.27,0.21, and 0.13.

- Prior: $f_0 = f_1 = 1$, $a = 0.5$, $b = 5$

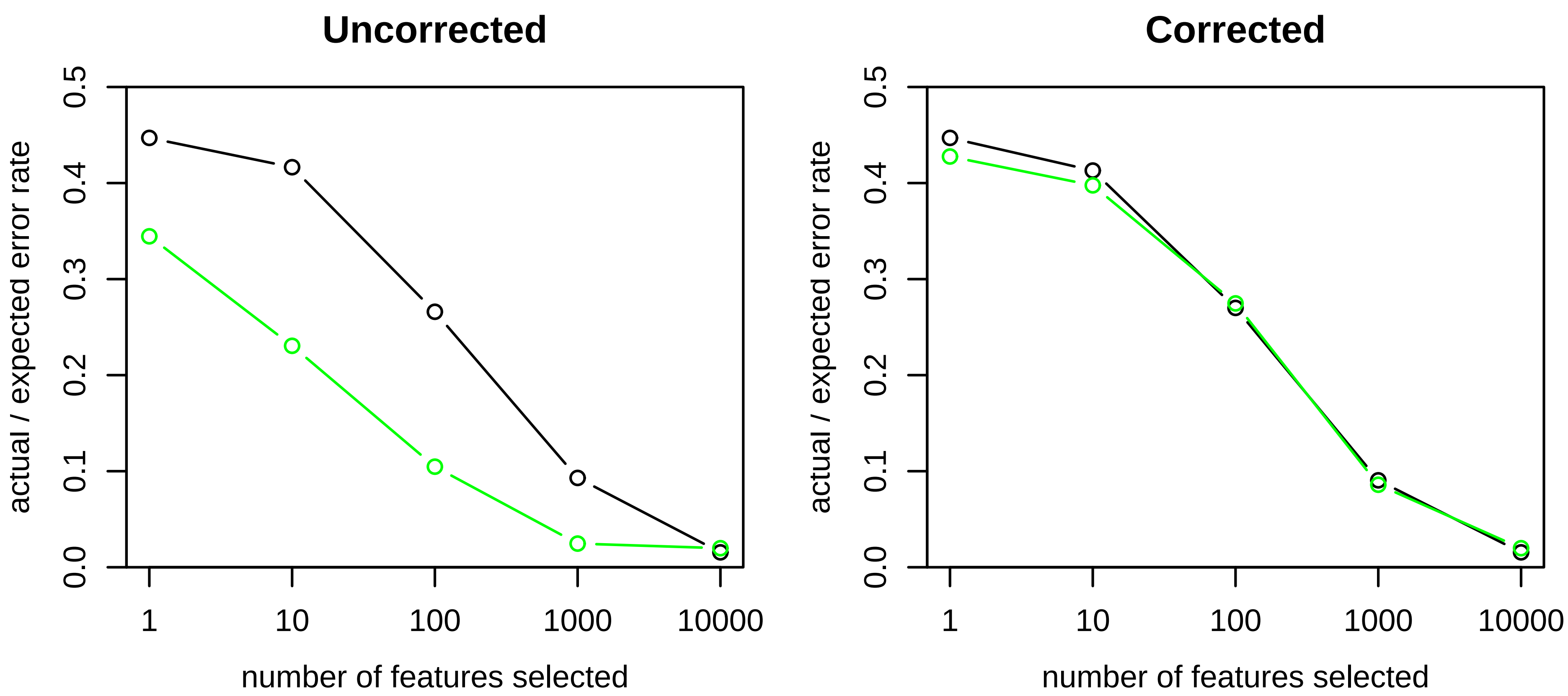
Looking into Feature Selection



Comparison of Actual and Expected Error Rates

Average Expected Error Rate:

$$(1/N)\sum_{i=1}^{N}\hat{p}^{(i)}\, I(\hat{p}^{(i)} < 1/2) + (1-\hat{p}^{(i)})\, I(\hat{p}^{(i)} \geq 1/2)$$



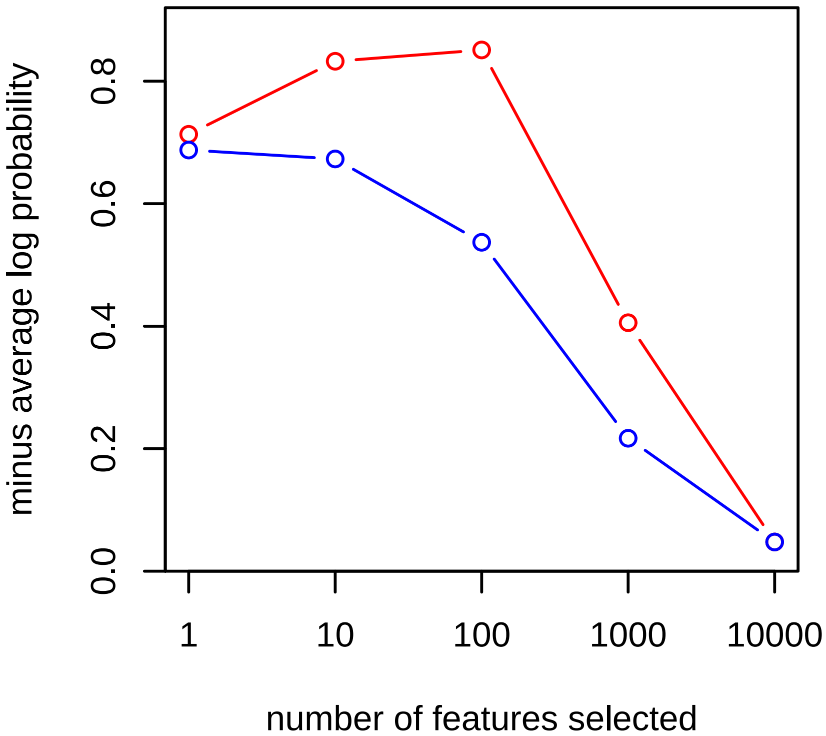
Comparison of Two Measures

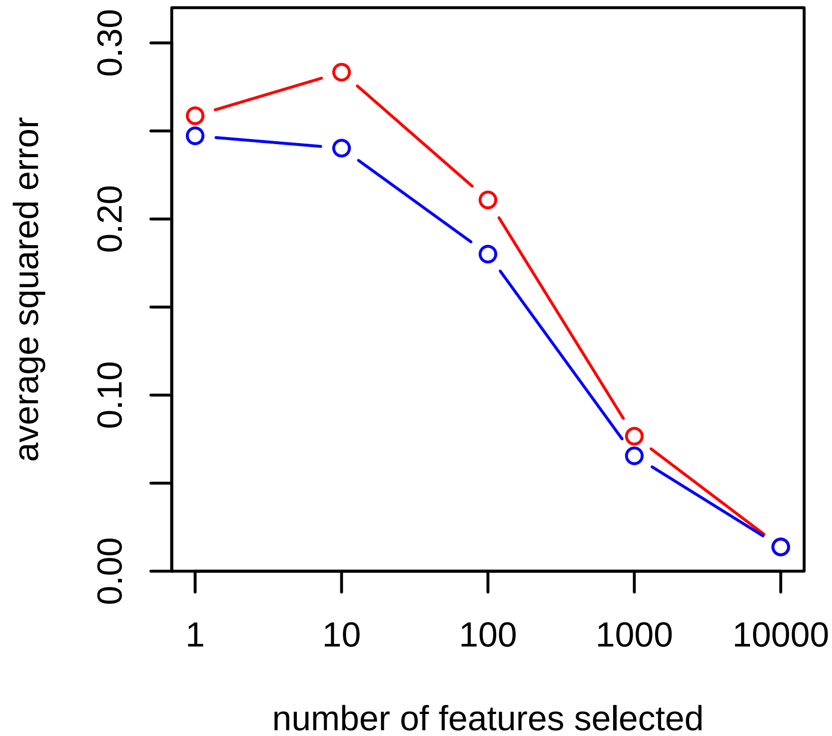
Average Minus Log Probability:

$$-(1/N)\sum_{i=1}^{N}[y^{(i)}\log(\hat{p}^{(i)}) + (1-y^{(i)})\log(1-\hat{p}^{(i)})]$$

Average Squared Error:

$$(1/N)\sum_{i=1}^{N}(y^{(i)} - \hat{p}^{(i)})^2$$

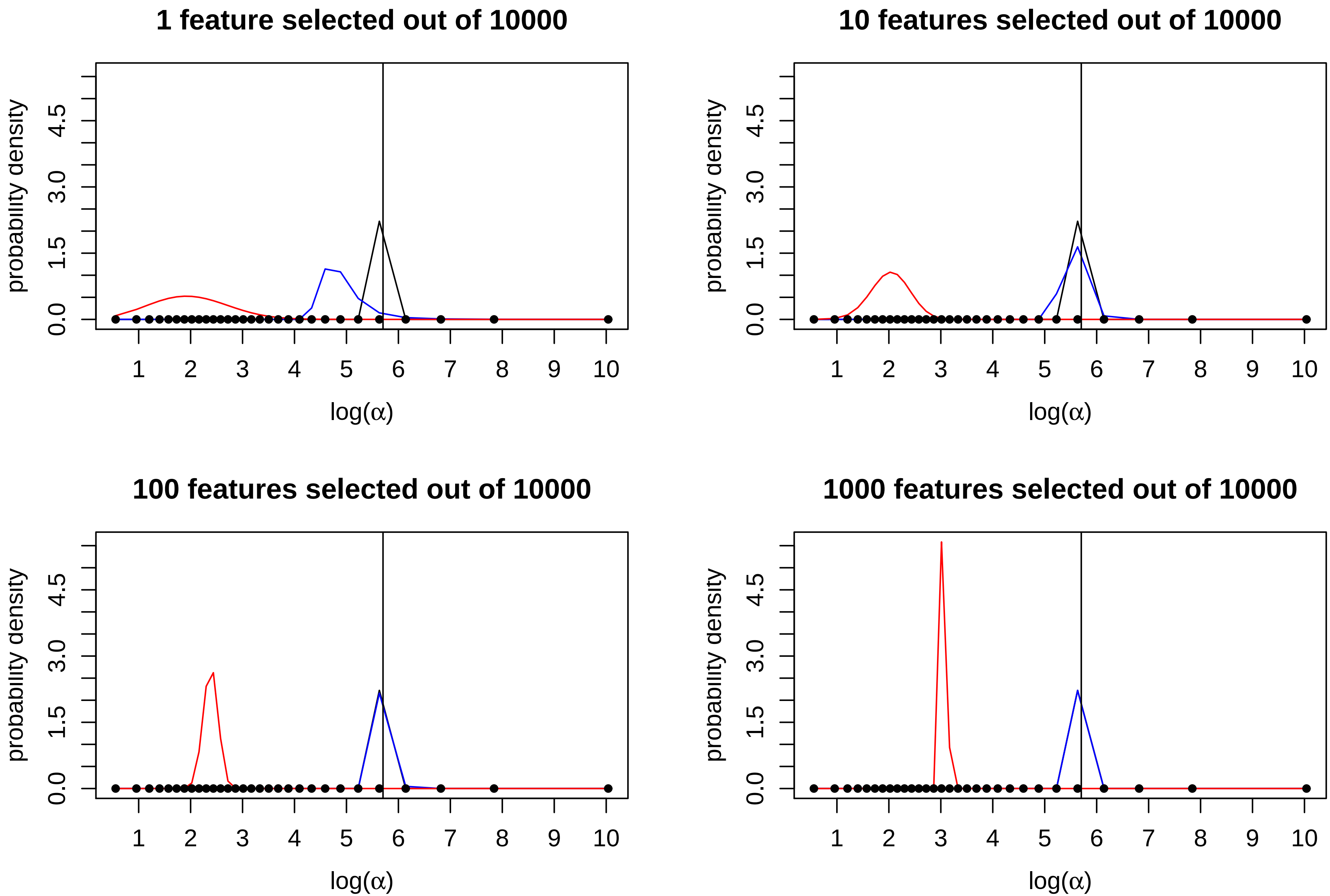




Comparison of Calibration for Predictions

	1000 features selected out of 10000					
	Corrected			Uncorrected		
Category	#	Pred	Actual	#	Pred	Actual
0.0 - 0.1	774	0.018	0.027	954	0.004	0.066
0.1 - 0.2	97	0.143	0.165	28	0.149	0.500
0.2 - 0.3	63	0.243	0.302	13	0.248	0.846
0.3 - 0.4	48	0.346	0.438	17	0.349	0.412
0.4 - 0.5	45	0.446	0.600	14	0.449	0.786
0.5 - 0.6	44	0.547	0.614	16	0.546	0.375
0.6 - 0.7	53	0.647	0.698	16	0.667	0.812
0.7 - 0.8	81	0.755	0.815	22	0.751	0.636
0.8 - 0.9	124	0.854	0.863	25	0.865	0.560
0.9 - 1.0	671	0.977	0.982	895	0.995	0.946

Posterior Distribution of $\log(\alpha)$



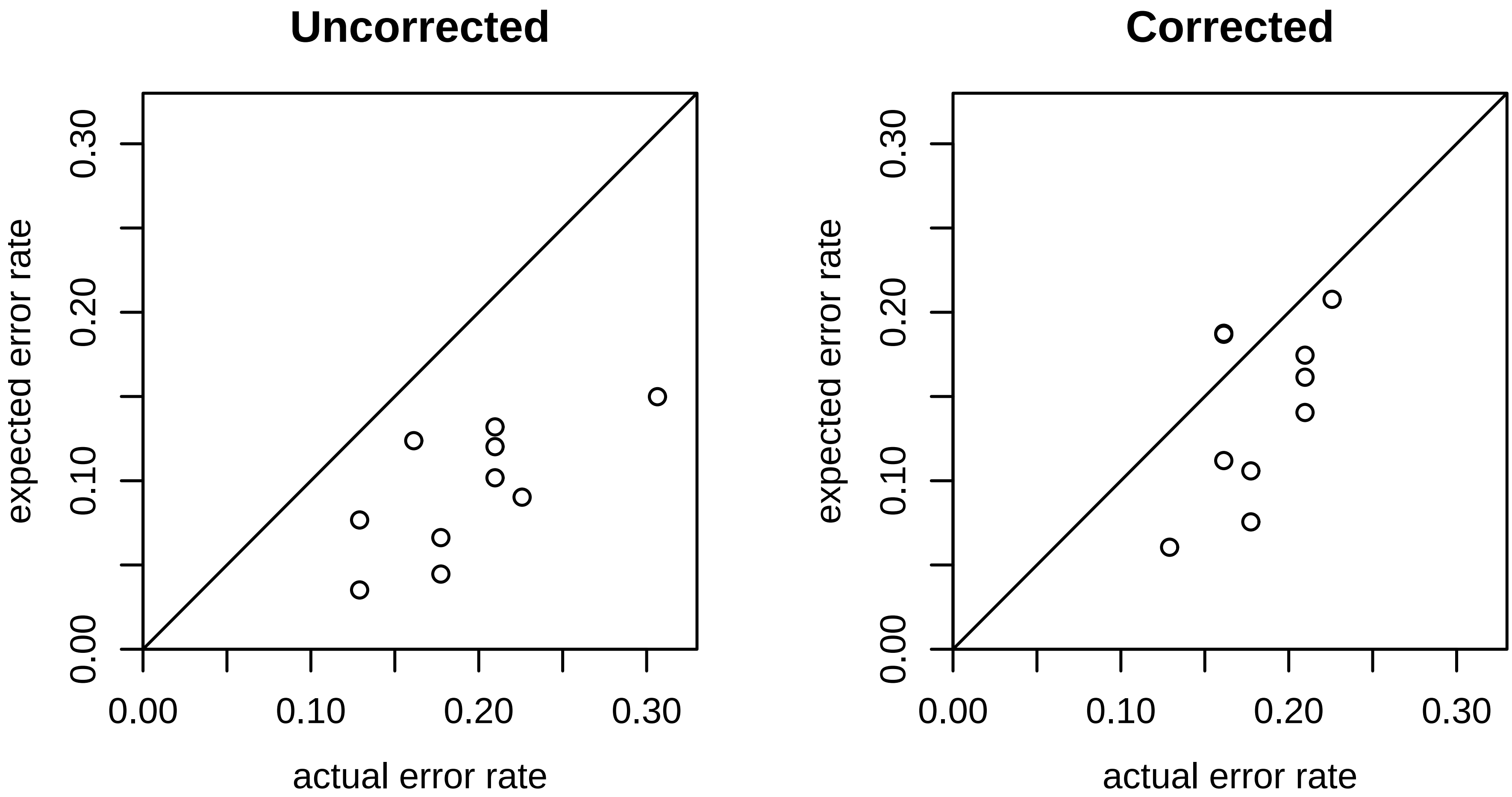
Computational Time

# of Features Selected	1	10	100	1000	10000
Uncorrected	12.66	28.80	203.60	2065.73	20627.71
Corrected	12.72	29.55	204.54	2076.21	

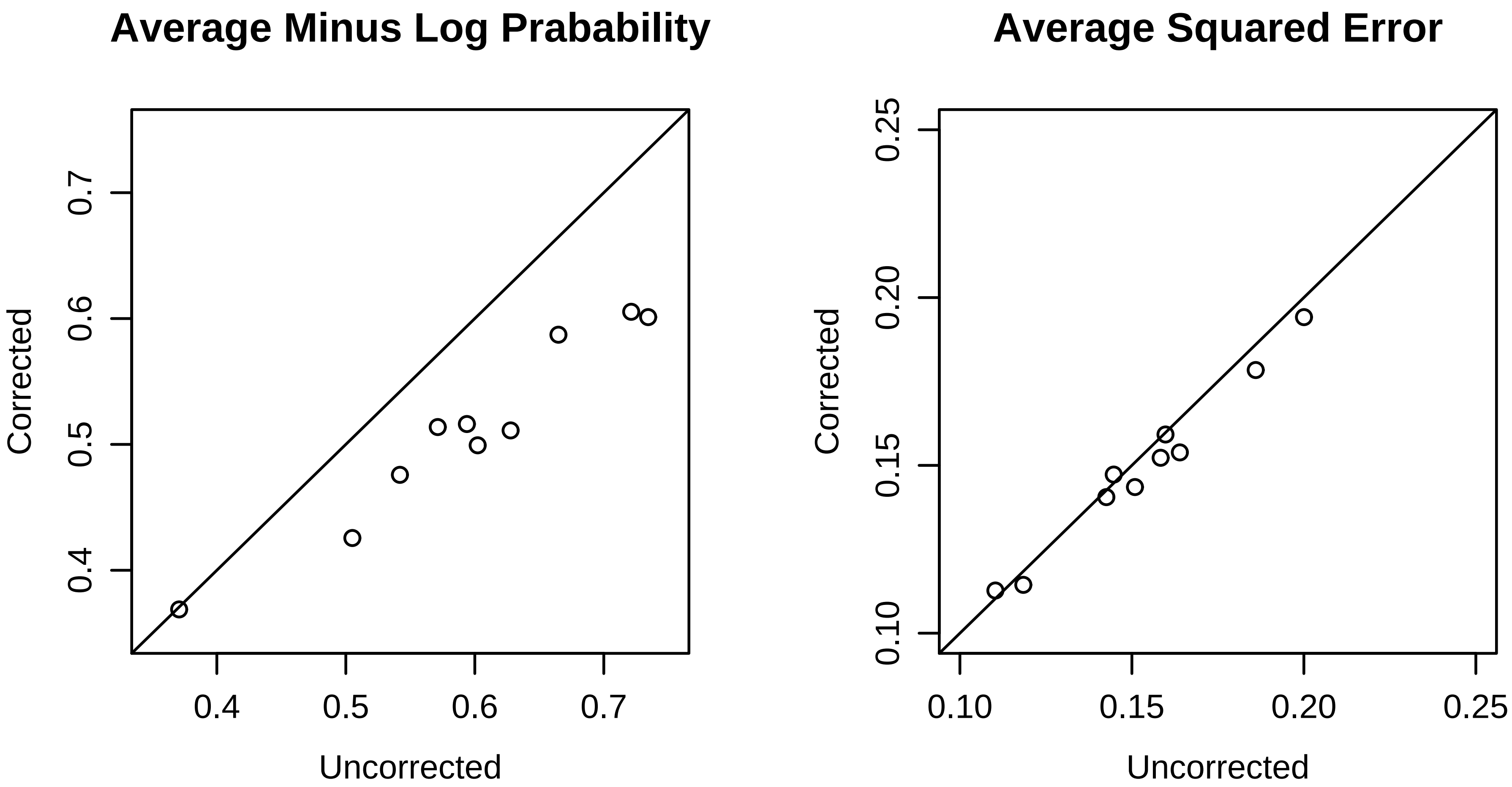
A Test with Gene Expression Data

- Data set: 2000 genes, 62 cases (40 Cancereous vs 22 Normal tissues)
- Converted into binary data by thresholding at medians of features
- Splited 2000 genes randomly into 10 subsets each with 200 genes.
- 5 Genes were selected out of 200 genes
- Used leave-one-out cross-validation to obtain predictive probabilities
- Prior the same as previous simulation experiment

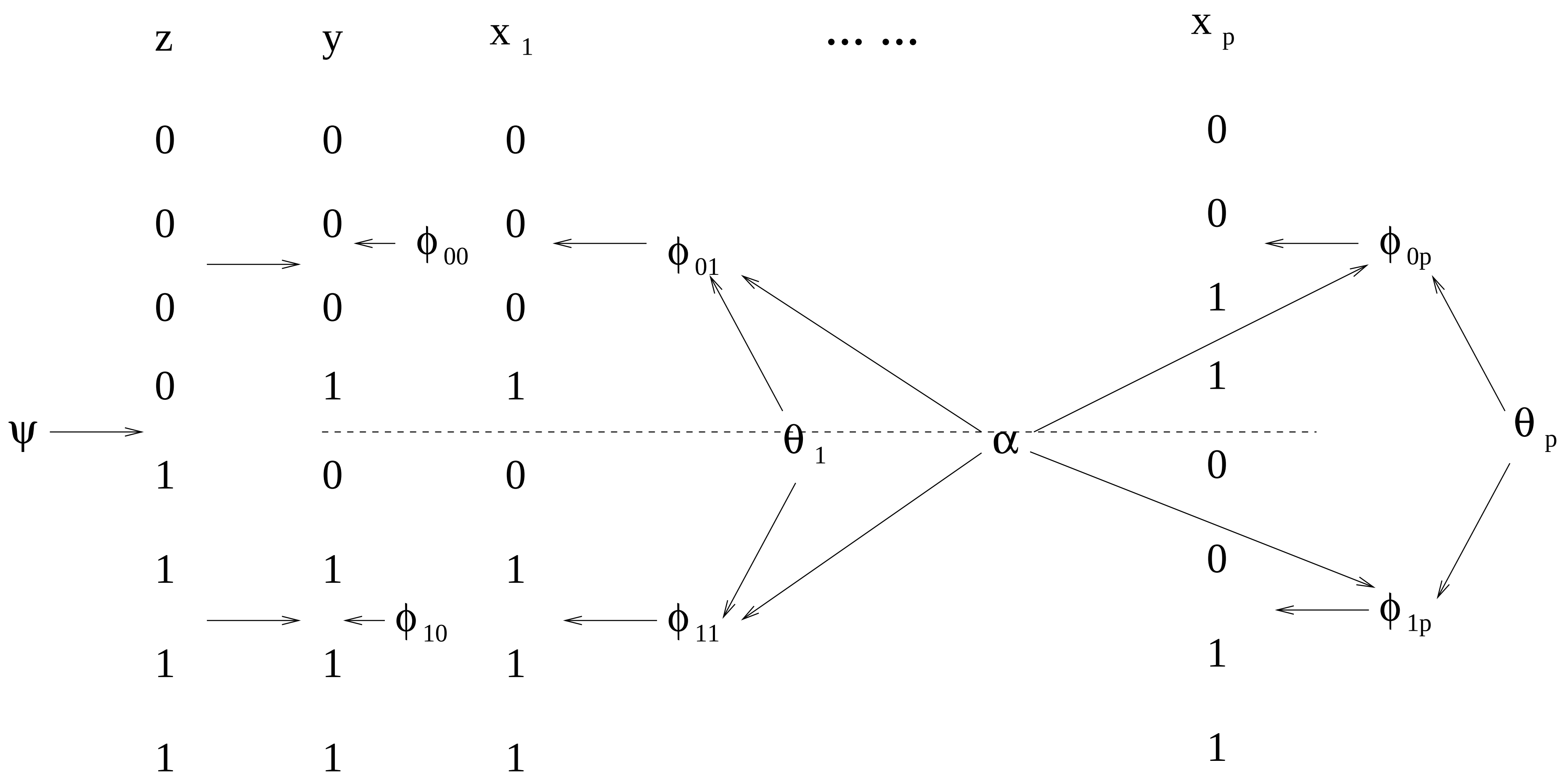
Comparison of Actual and Expected Error Rates



Comparison of Two Measures



Extended to Binary Mixture Models



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- One could extend the method to other models and other selection criteria.