

glmpathcr: An R Package for Ordinal Response Prediction in High-dimensional Data Settings

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Abstract

This paper describes an R package, **glmpathcr**, that provides a function for fitting a penalized continuation ratio model when interest lies in predicting an ordinal response. The function, `glmpath.cr` uses the coordinate descent fitting algorithm as implemented in `glmpath` and described by (Park and Hastie 2007a). Methods for extracting all estimated coefficients, extracting non-zero coefficient estimates, obtaining the predicted class, and obtaining the class-specific fitted probabilities have been implemented. Additionally, generic methods from `glmpath` including `summary`, `print`, and `plot` can be applied to a `glmpath.cr` object.

Keywords: ordinal response, penalized models, LASSO, L_1 constraint, R.

1. Introduction

High-throughput genomic experiments are frequently conducted for the purpose of examining whether genes are predictive of or significantly associated with phenotype. In many biomedical settings where histopathological or health status data are collected, phenotypic variables are recorded on an ordinal scale. Nevertheless, most often investigators neglect the ordinality of the phenotypic data and rather dichotomize the ordinal class then apply statistical methods suitable for two-class comparisons and predictions. This tendency to analyze ordinal data using dichotomous class methodologies may be due to the lack of available statistical methods and software for modeling an ordinal response in the presence of a high-dimensional covariate space. The approach of collapsing ordinal categories may neglect important information in the study (Armstrong and Sloan 1989).

A variety of statistical modeling procedures, namely, proportional odds, adjacent category, stereotype logit, and continuation ratio models can be used to predict an ordinal response. In this paper, we focus attention to the continuation ratio model because its likelihood can be easily re-expressed such that existing software can be readily used for model fitting. The backward formulation of the continuation ratio models the logit as

$$\log \left(\frac{P(Y = k|X = x)}{P(Y \leq k|X = x)} \right) = \alpha_k + \beta_k^T \mathbf{x} \quad (1)$$

whereas the forward formulation models the logit as

$$\log \left(\frac{P(Y = k|X = x)}{P(Y \geq k|X = x)} \right) = \alpha_k + \beta_k^T \mathbf{x}. \quad (2)$$

Rather than describe both formulations in detail, here we present the backward formulation, which is commonly used when progression through disease states from none, mild, moderate, severe is represented by increasing integer values, and interest lies in estimating the odds of more severe disease compared to less severe disease (Bender and Benner 2000). Suppose each observation, $i = 1, \dots, n$, belongs to one ordinal class $k = 1, \dots, K$. Therefore for $i = 1, \dots, n$ we can construct a vector \mathbf{y}_i to represent ordinal class membership, such that $\mathbf{y}_i = (y_{i1}, y_{i2}, \dots, y_{iK})^T$, where $y_{ik} = 1$ if the response is in category k and 0 otherwise, so that $n_i = \sum_{k=1}^K y_{ik} = 1$. Using the logit link, the equation representing the conditional probability for class k is

$$\delta_k(x) = P(Y = k | Y \leq k, X = x) = \frac{\exp(\alpha_k + \beta^T \mathbf{X})}{1 + \exp(\alpha_k + \beta^T \mathbf{X})}. \quad (3)$$

The likelihood for the continuation ratio model is then the product of conditionally independent binomial terms (Cox 1975), which is given by

$$L(\beta | \mathbf{y}, \mathbf{x}) = \prod_{i=1}^n \delta_2^{y_{i2}} (1 - \delta_2)^{n_i - \sum_{k=2}^K y_{ik}} \delta_3^{y_{i3}} (1 - \delta_3)^{n_i - \sum_{k=3}^K y_{ik}} \times \dots \times \delta_K^{y_{iK}} (1 - \delta_K)^{n_i - y_{iK}} \quad (4)$$

where here we have simplified our notation by not explicitly including the dependence of the conditional probability δ_k on \mathbf{x} . Further, simplifying our notation to let β represent the vector containing both the thresholds $(\alpha_2, \dots, \alpha_K)$ and the log odds $(\beta_1, \dots, \beta_p)$ for all $K - 1$ logits, the full parameter vector is

$$\beta = (\alpha_2, \beta_{21}, \beta_{22}, \dots, \beta_{2p}, \alpha_3, \beta_{31}, \beta_{32}, \dots, \beta_{3p}, \alpha_K, \beta_{K,1}, \beta_{K,2}, \dots, \beta_{K,p})^T \quad (5)$$

which is of length $(K - 1)(p + 1)$. As can be seen from equation 4, the likelihood can be factored into $K - 1$ independent likelihoods, so that maximization of the independent likelihoods will lead to an overall maximum likelihood estimate for all terms in the model (Bender and Benner 2000). Typically, to promote parsimony and interpretation, the model is constrained such that for each of the $K - 1$ vectors, $(\beta_{k1}, \beta_{k2}, \dots, \beta_{kp})$, are equal, thus yielding a constrained continuation ratio model.

2. Penalized Models

For datasets where the number of covariates p exceeds the sample size n , the backwards stepwise procedure cannot be undertaken. Furthermore, for any problem using a forward selection procedure the discrete variable inclusion process can exhibit high variance. Moreover, for high-dimensional covariate spaces, the best subset procedure is computationally prohibitive. Two penalized methods, ridge and L_1 penalization, places a penalty on a function of the coefficient estimates, thereby permitting a model fit even for high-dimensional data Tibshirani (1996, 1997). A generalization of these penalized models can be expressed as,

$$\tilde{\beta} = \arg \min_{\beta} \left(\sum_{i=1}^n (y_i - \beta_0 - \sum_{j=1}^p x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^p |\beta_j|^q \right) \quad (6)$$

for $q \geq 0$. When $q = 1$ we have the an L_1 penalized model, when $q = 2$ we have ridge regression. Values of $q \in (1, 2)$ provide a compromise between the L_1 and ridge penalized

models. Because when $q > 1$ coefficients are no longer set exactly equal to 0, the elastic net penalty was introduced

$$\lambda \sum_{j=1}^p (\alpha \beta_j^2 + (1 - \alpha) |\beta_j|). \quad (7)$$

3. Implementation

The **glmpathcr** package was written in the R programming environment (R Development Core Team 2009) and depends on the **glmpath** package (Park and Hastie 2007b). Similar to the **Design** package which includes a function **cr.setup** for restructuring a dataset for fitting a forward continuation ratio model, in this package the model is fit by restructuring the dataset then passing the restructured dataset to a penalized logistic regression fitting function. However, unlike **cr.setup** which produces an object of class **list** from which the response and restructured independent variables are extracted and passed to a model fitting algorithm, in the **glmpathcr** package the restructuring functions are transparent to the user. Specifically, the **glmpathcr** package fits either a forward or backward (default) penalized constrained continuation ratio model by specification of **method="forward"** in the **glmpath.cr** call. The **glmpath.cr** function restructures the dataset to represent the $K - 1$ conditionally independent likelihoods and then fits the penalized continuation ratio model using the **glmpath** framework. Therefore, the coordinate descent fitting procedure used by the **glmpath** function in the **glmpath** package are used in fitting the penalized continuation ratio model when invoking **glmpath.cr**. This allows fitting a penalized model for situations where the number of covariates p exceed the sample size n . In addition, methods for extracting the best fitting model from the path using AIC and BIC criteria, obtaining predicted class and fitted class probabilities, and returning coefficient estimates were written in addition to the **print**, **summary**, and **plot** methods copied from **glmpath**.

4. Example

A simulated dataset, **data**, consisting of 1,000 covariates and a three-class ordinal response with 30 observations in each class is included in the **glmpath** package for testing ordinal classification methodologies. The first column (**V1**) is stochastically associated with the ordinal response: for class 0, **V1** is distributed as $N(0,1)$; for class 1, **V1** is distributed as $N(1.5,1)$; and for class 2, **V1** is distributed as $N(3,1)$. All other predictor variables (**V2-V1000**) are multivariable normally distributed with mean vector **0** and variance-covariance matrix **I**. Therefore the Bayes Error associated with this dataset is 0.302. The last column in **data** is the ordinal response, **class**. The code for fitting a backward (default) continuation ratio model is given by

```
> library(glmpathcr)
> data(data)
> x <- data[, 1:1000]
> y <- data$class
> fit <- glmpath.cr(x, y)
```

As with `glmpath` model objects, methods such as `summary` and `plot` can be applied to `glmpath.cr` model objects, which are helpful for selecting the step at which to select the final model from the solution path.

```
> summary(fit)
```

	Df	Deviance	AIC	BIC
Step 1	3	1.977502e+02	203.7502	212.7821
Step 7	4	1.268914e+02	134.8914	146.9339
Step 9	6	1.236720e+02	135.6720	153.7358
Step 10	7	1.235747e+02	137.5747	158.6492
Step 12	8	1.229605e+02	138.9605	163.0455
Step 13	9	1.213437e+02	139.3437	166.4394
Step 15	10	1.206910e+02	140.6910	170.7974
Step 16	11	1.206072e+02	142.6072	175.7241
Step 18	12	1.185045e+02	142.5045	178.6321
Step 19	13	1.140777e+02	140.0777	179.2160
Step 21	14	1.059049e+02	133.9049	176.0538
Step 23	15	1.052149e+02	135.2149	180.3744
Step 25	16	1.025033e+02	134.5033	182.6735
Step 27	17	9.788337e+01	131.8834	183.0642
Step 29	18	9.250006e+01	128.5001	182.6915
Step 31	19	8.937950e+01	127.3795	184.5816
Step 32	20	8.936458e+01	129.3646	189.5773
Step 34	21	8.913574e+01	131.1357	194.3591
Step 35	22	8.740808e+01	131.4081	197.6421
Step 37	23	8.391957e+01	129.9196	199.1642
Step 39	24	8.211261e+01	130.1126	202.3679
Step 41	25	7.883779e+01	128.8378	204.1037
Step 43	26	7.744341e+01	129.4434	207.7199
Step 45	27	7.552956e+01	129.5296	210.8167
Step 47	28	7.464407e+01	130.6441	214.9419
Step 49	29	7.331620e+01	131.3162	218.6246
Step 50	30	7.128100e+01	131.2810	221.6001
Step 52	31	7.032096e+01	132.3210	225.6506
Step 54	32	6.973133e+01	133.7313	230.0717
Step 56	33	6.955485e+01	135.5548	234.9058
Step 58	34	6.941267e+01	137.4127	239.7743
Step 60	35	6.655017e+01	136.5502	241.9224
Step 62	36	6.591471e+01	137.9147	246.2976
Step 64	37	6.396196e+01	137.9620	249.3555
Step 67	38	5.591195e+01	131.9120	246.3161
Step 70	39	4.964509e+01	127.6451	245.0599
Step 73	40	4.588916e+01	125.8892	246.3146
Step 75	41	4.518095e+01	127.1809	250.6170
Step 77	42	4.439213e+01	128.3921	254.8388
Step 80	43	4.097572e+01	126.9757	256.4330

Step 82	44	3.855674e+01	126.5567	259.0247
Step 84	45	3.771496e+01	127.7150	263.1935
Step 86	46	3.683175e+01	128.8317	267.3210
Step 88	47	3.561162e+01	129.6116	271.1115
Step 90	48	3.533279e+01	131.3328	275.8433
Step 91	48	3.389858e+01	129.8986	274.4091
Step 93	48	3.248141e+01	128.4814	272.9919
Step 95	49	3.148533e+01	129.4853	277.0065
Step 96	49	3.115469e+01	129.1547	276.6758
Step 98	49	2.906390e+01	127.0639	274.5850
Step 101	50	2.708599e+01	127.0860	277.6178
Step 103	51	2.597671e+01	127.9767	281.5191
Step 105	52	2.523697e+01	129.2370	285.7900
Step 107	53	2.454167e+01	130.5417	290.1053
Step 110	54	2.252000e+01	130.5200	293.0943
Step 111	55	2.248267e+01	132.4827	298.0676
Step 114	56	1.674256e+01	128.7426	297.3381
Step 116	57	1.643027e+01	130.4303	302.0365
Step 119	58	1.221607e+01	128.2161	302.8329
Step 121	59	1.160682e+01	129.6068	307.2343
Step 122	59	1.048302e+01	128.4830	306.1105
Step 124	59	1.036497e+01	128.3650	305.9925
Step 126	60	9.736097e+00	129.7361	310.3742
Step 129	61	8.882654e+00	130.8827	314.5314
Step 130	61	8.367347e+00	130.3673	314.0161
Step 133	61	7.613208e+00	129.6132	313.2620
Step 136	62	6.748127e+00	130.7481	317.4075
Step 139	63	5.756419e+00	131.7564	321.4264
Step 141	64	5.720197e+00	133.7202	326.4009
Step 144	65	4.672943e+00	134.6729	330.3642
Step 147	66	4.320249e+00	136.3202	335.0222
Step 152	67	2.735014e+00	136.7350	338.4476
Step 155	68	1.247403e+00	137.2474	341.9706
Step 158	69	9.716167e-01	138.9716	346.7055
Step 162	70	5.010593e-01	140.5011	351.2455
Step 165	71	3.818247e-01	142.3818	356.1369
Step 166	70	3.476473e-01	140.3476	351.0921
Step 170	70	8.522756e-02	140.0852	350.8297
Step 173	71	6.081049e-02	142.0608	355.8159
Step 174	71	3.708819e-02	142.0371	355.7922
Step 176	71	3.342187e-02	142.0334	355.7885
Step 177	71	2.938603e-02	142.0294	355.7845
Step 179	71	2.541967e-02	142.0254	355.7805
Step 180	72	1.844144e-02	144.0184	360.7842
Step 182	73	1.449531e-02	146.0145	365.7909
Step 183	74	1.278486e-02	148.0128	370.7998
Step 184	74	1.264285e-02	148.0126	370.7997

Step 185	74	1.207392e-02	148.0121	370.7991
Step 186	74	1.180871e-02	148.0118	370.7988
Step 187	74	1.160685e-02	148.0116	370.7986
Step 188	74	8.075618e-03	148.0081	370.7951
Step 189	74	7.642540e-03	148.0076	370.7947
Step 190	74	7.474924e-03	148.0075	370.7945
Step 191	73	7.421659e-03	146.0074	365.7838
Step 192	73	6.660177e-03	146.0067	365.7830
Step 193	74	6.538656e-03	148.0065	370.7936
Step 194	75	6.202576e-03	150.0062	375.8038
Step 195	76	6.109357e-03	152.0061	380.8144
Step 196	78	5.805791e-03	156.0058	390.8354
Step 197	78	5.801257e-03	156.0058	390.8354
Step 198	77	5.601975e-03	154.0056	385.8245
Step 199	77	5.504980e-03	154.0055	385.8244
Step 200	77	5.245695e-03	154.0052	385.8242
Step 202	77	4.752132e-03	154.0048	385.8237
Step 203	78	4.656521e-03	156.0047	390.8342
Step 204	79	4.530401e-03	158.0045	395.8447
Step 206	80	4.305395e-03	160.0043	400.8551
Step 207	80	4.293758e-03	160.0043	400.8551
Step 209	80	3.787662e-03	160.0038	400.8546
Step 211	81	3.650458e-03	162.0037	405.8651
Step 212	82	3.453881e-03	164.0035	410.8755
Step 213	82	3.423946e-03	164.0034	410.8755
Step 214	81	3.383232e-03	162.0034	405.8648
Step 215	82	3.274787e-03	164.0033	410.8754
Step 216	82	3.013102e-03	164.0030	410.8751
Step 217	82	2.942978e-03	164.0029	410.8750
Step 218	84	2.832763e-03	168.0028	420.8962
Step 219	84	2.771885e-03	168.0028	420.8961
Step 220	85	2.697916e-03	170.0027	425.9067
Step 222	86	2.487565e-03	172.0025	430.9171
Step 223	87	2.437891e-03	174.0024	435.9277
Step 224	89	2.375010e-03	178.0024	445.9489
Step 225	90	2.328724e-03	180.0023	450.9595
Step 226	91	2.279899e-03	182.0023	455.9701
Step 227	90	2.245480e-03	180.0022	450.9594
Step 228	90	2.151490e-03	180.0022	450.9593
Step 229	92	2.121618e-03	184.0021	460.9806
Step 230	93	2.093159e-03	186.0021	465.9912
Step 231	93	2.062546e-03	186.0021	465.9911
Step 232	92	2.029814e-03	184.0020	460.9805
Step 233	91	1.970488e-03	182.0020	455.9698
Step 234	91	1.919379e-03	182.0019	455.9697
Step 235	92	1.896475e-03	184.0019	460.9803
Step 236	93	1.828767e-03	186.0018	465.9909

Step 237	93	1.825758e-03	186.0018	465.9909
Step 238	92	1.821194e-03	184.0018	460.9803
Step 239	91	1.808816e-03	182.0018	455.9696
Step 240	90	1.762903e-03	180.0018	450.9589
Step 241	91	1.709718e-03	182.0017	455.9695
Step 242	93	1.642881e-03	186.0016	465.9907
Step 243	95	1.604030e-03	190.0016	476.0120
Step 244	97	1.575597e-03	194.0016	486.0332
Step 245	99	1.531090e-03	198.0015	496.0544
Step 246	100	1.488077e-03	200.0015	501.0650
Step 247	100	1.465819e-03	200.0015	501.0650
Step 248	100	1.409207e-03	200.0014	501.0649
Step 249	103	1.369562e-03	206.0014	516.0968
Step 250	106	1.332009e-03	212.0013	531.1287
Step 251	106	1.316473e-03	212.0013	531.1287
Step 252	106	1.312051e-03	212.0013	531.1287
Step 253	105	1.302143e-03	210.0013	526.1180
Step 254	104	1.298270e-03	208.0013	521.1074
Step 255	103	1.277893e-03	206.0013	516.0967
Step 256	104	1.243826e-03	208.0012	521.1073
Step 257	106	1.224708e-03	212.0012	531.1286
Step 258	106	1.211353e-03	212.0012	531.1286
Step 259	108	1.189521e-03	216.0012	541.1498
Step 260	109	1.149689e-03	218.0011	546.1604
Step 261	111	1.117974e-03	222.0011	556.1816
Step 262	112	1.107710e-03	224.0011	561.1923
Step 263	112	1.077822e-03	224.0011	561.1922
Step 264	113	1.067414e-03	226.0011	566.2029
Step 265	118	1.046297e-03	236.0010	591.2560
Step 266	119	1.040973e-03	238.0010	596.2666
Step 267	118	1.040083e-03	236.0010	591.2560
Step 268	118	1.021432e-03	236.0010	591.2560
Step 269	118	1.011200e-03	236.0010	591.2560
Step 271	117	9.713459e-04	234.0010	586.2453
Step 272	117	9.558112e-04	234.0010	586.2453
Step 273	117	9.164918e-04	234.0009	586.2452
Step 274	121	8.957896e-04	242.0009	606.2878
Step 275	124	8.861962e-04	248.0009	621.3197
Step 276	128	8.771551e-04	256.0009	641.3622
Step 277	129	8.600954e-04	258.0009	646.3728
Step 278	130	8.366869e-04	260.0008	651.3834
Step 279	135	8.173980e-04	270.0008	676.4366
Step 280	136	8.038641e-04	272.0008	681.4472
Step 281	138	7.826633e-04	276.0008	691.4685
Step 282	140	7.259221e-04	280.0007	701.4897
Step 284	143	6.836433e-04	286.0007	716.5215

```
> plot(fit, xvar = "step", type = "bic", plot.all.steps = TRUE,
+      breaks = FALSE)
```

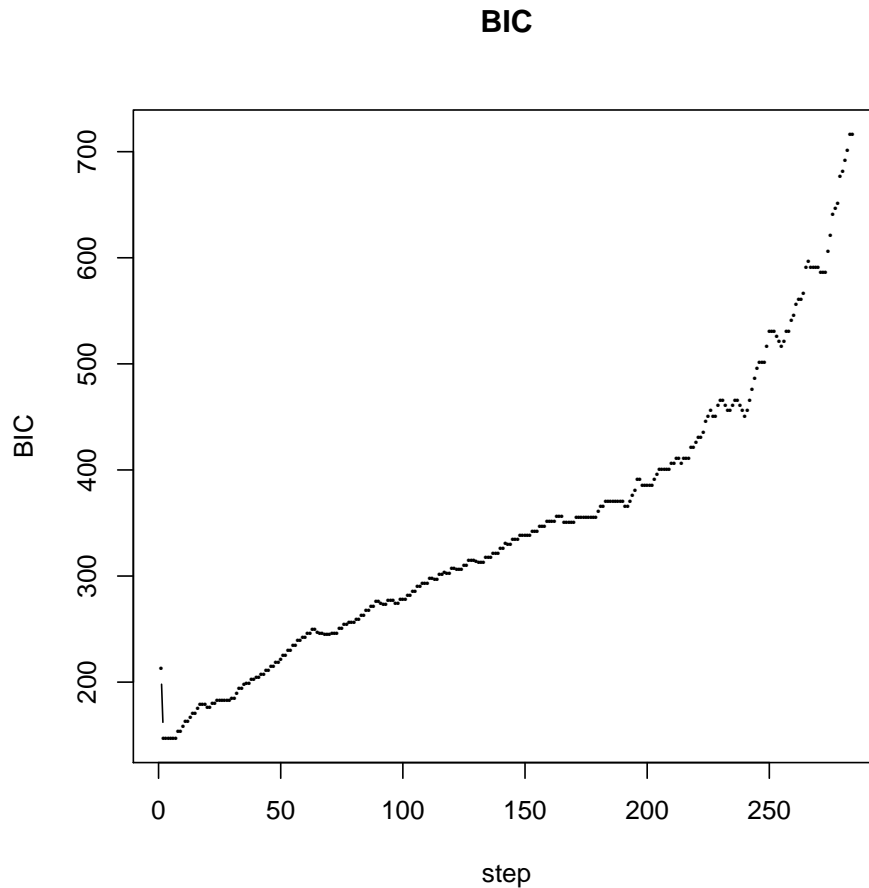


Figure 1: Plot of regularization path for `glm path.cr` object using simulated dataset, `data`.

Note that when plotting, the horizontal axis can be `norm`, `lambda`, or `step`, however extractor functions for `glm path.cr` generally require the step to be selected, so we have selected `xvar = "step"` in this example. The vertical axis can be coefficients, `aic` or `bic`. As one can see, there is a multitude of models fit from one call to `glm path.cr`. To facilitate extraction of best fitting models using commonly used criterion, the `model.select` function can be used. The `model.select` function extracts the best fitting model from the solution path, where the `which` parameter allows one to select either AIC or by default, BIC.

```
> BIC.step <- model.select(fit)
> BIC.step
```

```
[1] 7
```

In this example, Step 7 corresponds to a 4 degree of freedom model having the minimum BIC of 146.9339.

The `coef` function returns all estimated coefficients for a `glmpath.cr` fitted model, where the model selected is indicated by step `s`. The `nonzero.coef` function returns only those non-zero coefficient estimates for a selected model.

```
> coefficients <- coef(fit, s = BIC.step)
> sum(coefficients != 0)
```

```
[1] 6
```

```
> nonzero.coef(fit, s = BIC.step)
```

Intercept	V1	V285	V497	cp1
-1.3797425221	0.8460541902	-0.0040386156	0.0001098907	0.7940460195
cp2				
-0.7940460865				

Note that the `glmpath.cr` function fits a penalized constrained continuation ratio model; therefore for K classes, there will be $K - 1$ intercepts representing the cutpoints between adjacent classes. In this package, the nomenclature for these cutpoints is to use "cp k " where $k = 1, \dots, K - 1$. In this dataset, $K = 3$ so the intercepts are `cp1` and `cp2` with `Intercept` being an offset. When using the BIC to select the final model, the only variables having a non-zero coefficient estimate are the truly important covariate `V1` along with two noise covariates `V285` and `V497`.

Continuation ratio models predicts conditional probabilities so a new method to extract the fitted probabilities and predicted class was created. The `predict` and `fitted` functions are equivalent, and return either the predicted class or the fitted probabilities from the penalized continuation ratio model for a `glmpath.cr` object. The user is required to supply the fitted `glmpath.cr` model object, a data matrix `newx` that is either the same as the training data or an independent dataset having the same number and order of covariates as the training data, a vector `newy` that provides the class labels of the ordinal response. These functions extract the fitted values for the best fitting model using the BIC criteria by default, which can be changed to extracting the best fitting AIC model by supplying `which="AIC"`. By default, the predicted class is output. If one desired the fitted class-specific probabilities from the model, the `type="probs"` argument should be supplied.

```
> pred <- predict(fit)
> table(pred, y)
```

	y			
pred	0	1	2	
1	25	7	0	
2	5	18	8	
3	0	5	22	

```
> pred <- predict(fit, which = "AIC", type = "probs")
> pred[1:10, ]
```

	0	1	2
[1,]	0.8824815	0.11378793	0.0037305240
[2,]	0.4956481	0.47715531	0.0271965511
[3,]	0.9737725	0.02546851	0.0007589597
[4,]	0.9282863	0.06954289	0.0021708481
[5,]	0.8861740	0.11022681	0.0035991901
[6,]	0.9508358	0.04770922	0.0014550130
[7,]	0.7375813	0.25257227	0.0098464754
[8,]	0.7677757	0.22382923	0.0083950557
[9,]	0.6868516	0.30059848	0.0125499351
[10,]	0.6447785	0.34013329	0.0150882334

Typically an unbiased estimate of error is desired. In this case, we can simulate a test dataset following the same procedure that was used to generate the original training set data. Afterward, we can apply the original model fit to the test set for estimating error. The `set.seed` function is used only to permit others to replicate these results.

```
> library(mvtnorm)
> set.seed(9)
> class1 <- rmvnorm(30, mean = rep(0, 1000), sigma = diag(1, nrow = 1000))
> class2 <- rmvnorm(30, mean = c(1.5, rep(0, 999)), sigma = diag(1,
+   nrow = 1000))
> class3 <- rmvnorm(30, mean = c(3, rep(0, 999)), sigma = diag(1,
+   nrow = 1000))
> class <- rep(0:2, each = 30)
> testset <- data.frame(cbind(rbind(class1, class2, class3), class))
> rm(class1, class2, class3, class)
> pred <- predict(fit, newx = testset[, 1:1000])
> table(pred, testset$class)
```

```
pred  0  1  2
     1 23 10  0
     2  6 13  9
     3  1  7 21
```

For illustrative purposes, a forward continuation ratio model can be fit using the syntax

```
> fit <- glmpath.cr(x, y, method = "forward")
```

and the predicted class can be obtained using

```
> pred <- predict(fit)
> table(pred, y)
```

```
      y
pred  0  1  2
     1 24  6  0
     2  6 19  7
     3  0  5 23
```

Summary

Herein we have described the **glmpathcr** package which works in conjunction with the **glmpath** package in the R programming environment. The package provides methods for fitting either a forward or backward penalized continuation ratio model. When applied to a simulated dataset having Bayes' error of 0.302, the method reported a test set error of 0.367. Moreover, the likelihood-based penalized continuation ratios models have been demonstrated to have good performance when applied to microarray gene expression datasets (Archer and Williams 2010) in comparison to corresponding penalized Bayesian continuation ratio models (Kiiveri 2008). Therefore the **glmpathcr** package should be helpful when predicting an ordinal response for datasets where the number of covariates exceeds the number of available samples.

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