ptLasso Vignette

Contents

1 Introduction to pretraining

Suppose we have a dataset spanning ten cancers and we want to fit a lasso penalized Cox model to predict survival time. Some of the cancer classes in our dataset are large (e.g. breast, lung) and some are small (e.g. head and neck). There are two obvious approaches: (1) fit a "pancancer model" to the entire training set and use it to make predictions for all cancer classes and (2) fit a separate (class specific) model for each cancer and use it to make predictions for that class only. Pretraining is a method that bridges these two options; it has a hyperparameter that allows you to fit the pancancer model, the class specific models, and everything in between.

`ptLasso` is a package that fits pretrained models using the `glmnet` package (Tay, Narasimhan, and Hastie (2023)), including lasso, elasticnet and ridge models .

Our example dataset consisting of ten different cancers is called **input grouped**. There is a grouping on the rows of X and each row belongs to one of the cancer classes. Alternatively, data can be **target grouped**, where there is no grouping on the rows of X, but we have (for example) a multinomial outcome. We could fit one multinomial model, or we could fit a set of one-vs-rest models. Pretraining again bridges the two approaches, and this is described in detail in the section "Target grouped data". The remainder of this introduction describes the input grouped setting.

Pretraining is a general method to pass information from one model to another – it has many uses beyond what has already been discussed here, including time series data, multi-response data with mixed response types, and multitask learning. Some of these modeling tasks are not supported by the `ptLasso` package, and this vignette shows how to do pretraining for them using the `glmnet` package.

Before we describe pretraining in more detail, we will first give a quick review of the lasso.

1.1 Review of the lasso

For the Gaussian family with data $(x_i, y_i), i = 1, 2, \ldots n$, the lasso has the form

$$\text{argmin}_{\beta_0,\beta} \frac{1}{2} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|. \tag{1}$$

Varying the regularization parameter $\lambda \geq 0$ yields a path of solutions: an optimal value $\hat{\lambda}$ is usually chosen by cross-validation, using for example the `cv.glmnet` function from the package `glmnet`.

In GLMs and ℓ_1-~regularized GLMs, one can include an *offset*: a pre-specified n-vector that is included as an additional column to the feature matrix, but whose weight β_j is fixed at 1. Secondly, one can generalize the ℓ_1 norm to a weighted norm, taking the form

$$\sum_j \text{pf}_j |\beta_j| \tag{2}$$

where each $\text{pf}_j \geq 0$ is a **penalty factor** for feature j. At the extremes, a penalty factor of zero implies no penalty and means that the feature will always be included in the model; a penalty factor of $+\infty$ leads to that feature being discarded (i.e., never entered into the model).

1.2 Details of pretraining

Pretraining model fitting happens in two steps. First, train a model using the full data:

$$\hat{\mu}_0, \hat{\theta}_2, \ldots, \hat{\theta}_K, \hat{\beta}_0 = \arg \min_{\mu,\theta_1,\ldots,\theta_{k-1},\beta} \frac{1}{2} \sum_{k=1}^{K} \|y_k - (\mu \mathbf{1} + \theta_k \mathbf{1} + X_k \beta)\|_2^2 + \lambda ||\beta||_1, \tag{3}$$

where:

- X_k, y_k are the observations in group k,

- θ_k is the group specific intercept for group k (by convention, $\hat{\theta}_1 = 0$),
- μ, β are the overall intercept and coefficients,
- and λ is a hyperparameter that has been chosen (perhaps the value minimizing the CV error).

Define $S(\hat{\beta}_0)$ to be the support set (the nonzero coefficients) of $\hat{\beta}_0$.

Then, for each group k, fit an *individual* model: find $\hat{\beta}_k$ and $\hat{\mu}_k$ such that

$$\hat{\mu}_k, \hat{\beta}_k = \arg\min_{\mu,\beta} \frac{1}{2}\|y_k - (1-\alpha)\left(\hat{\mu}_0\mathbf{1} + \hat{\theta}_k\mathbf{1} + X_k\hat{\beta}_0\right) - (\mu\mathbf{1} + X_k\beta)\|_2^2 + \lambda\sum_{j=1}^{p}\left[I(j \in S(\hat{\beta}_0)) + \frac{1}{\alpha}I(j \notin S(\hat{\beta}_0))\right]|\beta_j|, \quad (4)$$

where $\lambda > 0$ and $\alpha \in [0, 1]$ are hyperparameters that may be chosen through cross validation.

Note that this is a lasso linear regression model with *offset* $(1-\alpha)\left(\hat{\mu}_0\mathbf{1} + \hat{\theta}_k\mathbf{1} + X_k\hat{\beta}_0\right)$ and coefficient j has *penalty factor* 1 if $j \in S(\hat{\beta}_0)$ and $\frac{1}{\alpha}$ otherwise.

Notice that when $\alpha = 0$, this returns the overall model fine tuned for each group: this second stage model is only allowed to fit the residual $y_k - \left(\hat{\mu}_0\mathbf{1} + \hat{\theta}_k\mathbf{1} + X_k\hat{\beta}_0\right)$, and the penalty factor $I(j \in S(\hat{\beta}_0)) + \infty I(j \notin S(\hat{\beta}_0))$ disallows the use of β_j unless it was already selected by the overall model.

At the other extreme, when $\alpha = 1$, this is equivalent to fitting a separate model for each class. There is no offset, and the lasso penalty is 1 for all features (the usual lasso penalty).

1.3 `ptLasso` under the hood

All model fitting in `ptLasso` is done with `cv.glmnet`. The first step of pretraining is a straightforward call to `cv.glmnet`; the second step is done by calling `cv.glmnet` with:

1.`offset` $(1-\alpha)\left(\hat{\mu_0}\mathbf{1} + X_k\hat{\beta}_0\right)$ and 2.`penalty.factor`, the j^{th} entry of which is 1 if $j \in S(\hat{\beta}_0)$ and $\frac{1}{\alpha}$ otherwise.

Because `ptLasso` uses `cv.glmnet`, it inherits most of the virtues of the `glmnet` package: for example, it handles sparse input-matrix formats, as well as range constraints on coefficients.

Additionally, one call to `ptLasso` fits an overall model, pretrained class specific models, and class specific models for each group (without pretraining). The `ptLasso` package also includes methods for prediction and plotting, and a function that performs K-fold cross-validation.

2 Installation

To install this package, do the following.

```
require(remotes)
remotes::install_github("erincr/ptLasso")
```

3 Quick start

This section shows how to use the main functions in `ptLasso`. We will show more details and options in the following sections. First, we load the `ptLasso` package:

```
require(ptLasso)
#> Loading required package: ptLasso
#> Loading required package: ggplot2
#> Loading required package: glmnet
```

Table 1: Coefficients for simulating input grouped data

	1-10	11-20	21-30	31-40	41-59	51-60	61-120
group 1	3	3	0	0	0	0	0
group 2	6	0	3	0	0	0	0
group 3	9	0	0	3	0	0	0
group 4	12	0	0	0	3	0	0
group 5	15	0	0	0	0	3	0

```
#> Loading required package: Matrix
#> Loaded glmnet 4.1-8
#> Loading required package: gridExtra
```

To show how to use `ptLasso`, we'll simulate data with 5 groups and a continuous response using the helper function `gaussian.example.data`. There are $n = 200$ observations in each group and $p = 120$ features. All groups share 10 informative features; though the features are shared, they have different coefficient values. Each group has 10 additional features that are specific to that group, and all other features are uninformative. The coefficients for the 5 groups are in Table 1.

```
#> Loading required package: knitr
#> Loading required package: kableExtra
```

```
set.seed(1234)

out = gaussian.example.data()
x = out$x; y = out$y; groups = out$groups

outtest = gaussian.example.data()
xtest = outtest$x; ytest = outtest$y; groupstest = outtest$groups
```

Now we are ready to fit a model using `ptLasso`. We'll start by defining the pretraining hyperparamter $\alpha = 0.5$ (randomly chosen). In practice we recommend using a validation set to measure performance for a few different choices of α, or using `cv.ptLasso`, which will recommend a choice of α based on CV performance.

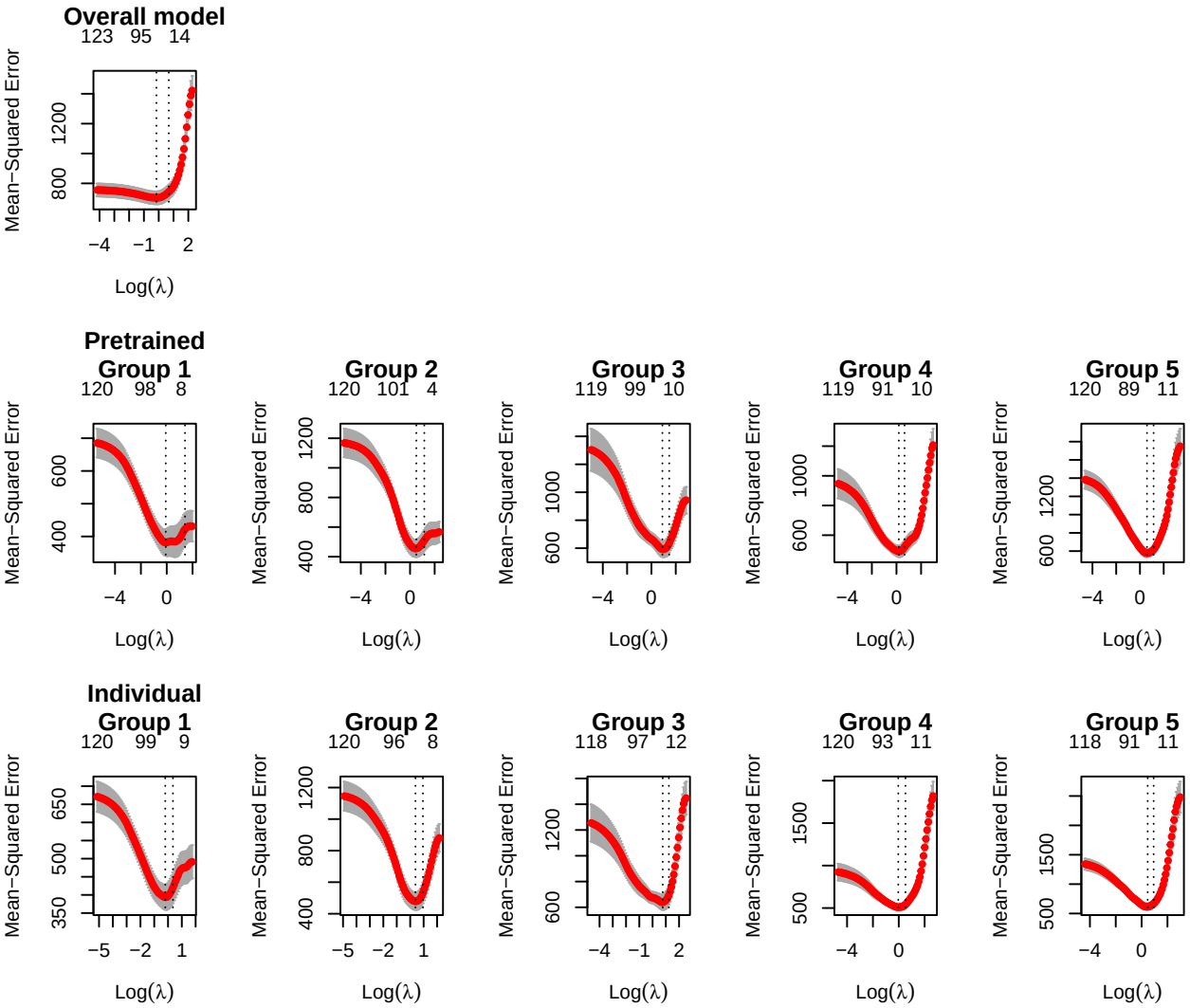
```
fit <- ptLasso(x, y, groups, alpha = 0.5)
```

The function `ptLasso` used `cv.glmnet` to fit 11 models:

- the *overall* model (using all 5 groups),
- the 5 *pretrained* models (one for each group) and
- the 5 *individual* models (one for each group).

A call to `plot` will show us the cross validation curves for each model. The top row shows the overall model, the middle row the pretrained models, and the bottom row the individual models.

```
plot(fit)
```



`predict` makes predictions from all 11 models. It returns a list containing:

1. `yhatoverall` (predictions from the overall model),
2. `yhatpre` (predictions from the pretrained models) and
3. `yhatind` (predictions from the individual models).

By default, `predict` uses `lambda.min` for all 11 `cv.glmnet` models; you could instead specify `s = lambda.1se` or use a numeric value. Whatever value of λ you choose will be used for all models (overall, pretrained and individual).

```
preds = predict(fit, xtest, groupstest=groupstest)
```

If you also provide `ytest` (e.g. for model validation), `predict` will additionally compute performance measures.

```
preds = predict(fit, xtest, groupstest=groupstest, ytest=ytest)
preds
#>
#> Call:
#> predict.ptLasso(fit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
```

```
#> alpha =  0.5
#>
#> Performance (Mean squared error):
#>
#>            allGroups  mean group_1 group_2 group_3 group_4 group_5    r^2
#> Overall        758.6 758.6   805.1   534.9   568.7   802.6  1081.5 0.5353
#> Pretrain       493.8 493.8   550.9   428.7   518.8   496.7   473.9 0.6975
#> Individual     532.8 532.8   584.1   443.2   567.2   550.5   518.9 0.6736
#>
#> Support size:
#>
#> Overall    47
#> Pretrain   98 (16 common + 82 individual)
#> Individual 109
```

To access the coefficients of the fitted models, use `coef` as usual. This returns a list with the coefficients of the individual models, pretrained models and overall models, as returned by `glmnet`.

```
all.coefs = coef(fit, s= "lambda.min")
names(all.coefs)
#> [1] "individual" "pretrain"   "overall"
```

The entries for the individual and pretrained models are lists with one entry for each group. Because we have 5 groups, we'll have 5 sets of coefficients.

```
length(all.coefs$pretrain)
#> [1] 5
```

The first few coefficients for group 1 from the pretrained model are:

```
head(all.coefs$pretrain[[1]])
#> 6 x 1 sparse Matrix of class "dgCMatrix"
#>                      s1
#> (Intercept)  0.44678793
#> V1          -3.96783783
#> V2           .
#> V3           .
#> V4          -0.09154089
#> V5          -0.85125296
```

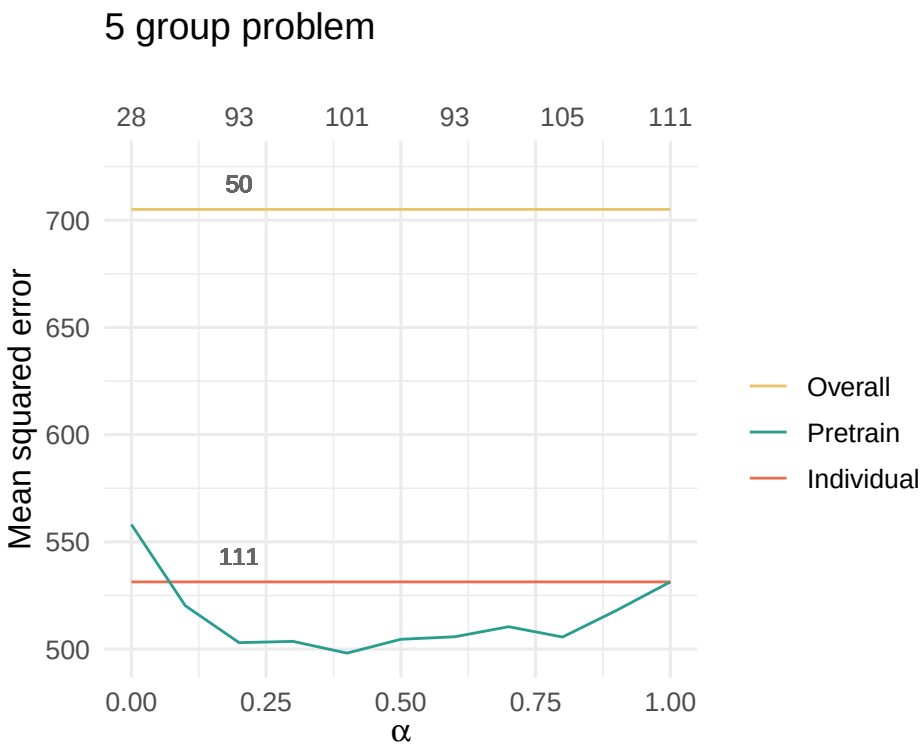
When we used `ptLasso` to fit a model, we chose $\alpha = 0.5$. If we want to use cross validation to compare many choices of α, we can use `cv.ptLasso`. After fitting, the `cv.ptLasso` object will print out the cross validated mean squared error for (1) the overall model, (2) the pretrained models for all compared choices of α and (3) the individual models.

```
cvfit <- cv.ptLasso(x, y, groups)
cvfit
#>
#> Call:
#> cv.ptLasso(x = x, y = y, groups = groups, family = "gaussian",
#>     type.measure = "mse", use.case = "inputGroups")
#>
#>
#>
#> type.measure:  mse
#>
#>
```

```
#>            alpha overall  mean wtdMean group_1 group_2 group_3 group_4 group_5
#> Overall             705.0 705.0   705.0   735.3   519.2   566.4   667.2  1037.0
#> Pretrain      0.0   558.1 558.1   558.1   474.8   516.3   607.1   563.4   629.0
#> Pretrain      0.1   520.2 520.2   520.2   417.0   470.7   620.7   511.4   581.4
#> Pretrain      0.2   503.0 503.0   503.0   410.1   464.6   608.2   486.1   545.9
#> Pretrain      0.3   503.6 503.6   503.6   427.1   478.2   571.2   479.6   561.8
#> Pretrain      0.4   498.1 498.1   498.1   377.1   464.1   582.7   496.3   570.4
#> Pretrain      0.5   504.6 504.6   504.6   376.9   478.6   590.5   500.7   576.3
#> Pretrain      0.6   505.7 505.7   505.7   382.9   467.0   616.8   493.8   568.2
#> Pretrain      0.7   510.4 510.4   510.4   398.9   482.5   603.3   471.3   596.1
#> Pretrain      0.8   505.6 505.6   505.6   378.5   483.7   593.7   502.6   569.5
#> Pretrain      0.9   518.0 518.0   518.0   419.3   485.9   596.8   518.3   569.8
#> Pretrain      1.0   531.3 531.3   531.3   416.2   509.3   613.9   509.4   607.9
#> Individual          531.3 531.3   531.3   416.2   509.3   613.9   509.4   607.9
#>
#> alphahat (fixed) = 0.4
#> alphahat (varying):
#> group_1 group_2 group_3 group_4 group_5
#>     0.5     0.4     0.3     0.7     0.2
```

We can plot the `cv.ptLasso` object to visualize performance as a function of α:

```
plot(cvfit)
```



And, as with `ptLasso`, we can `predict`. By default, `predict` uses the α that minimized the cross validated MSE:

```
preds = predict(cvfit, xtest, groupstest=groupstest, ytest=ytest)
preds
#>
#> Call:
```

```
#> predict.cv.ptLasso(cvfit = cvfit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
#> alpha =  0.4
#>
#> Performance (Mean squared error):
#>
#>            allGroups  mean group_1 group_2 group_3 group_4 group_5    r^2
#> Overall        757.1 757.1   815.7   542.6   567.1   792.7  1067.5 0.5362
#> Pretrain       501.9 501.9   585.7   439.0   519.4   494.7   470.6 0.6926
#> Individual     529.3 529.3   572.6   441.8   562.4   550.5   518.9 0.6758
#>
#> Support size:
#>
#> Overall    50
#> Pretrain   101 (20 common + 81 individual)
#> Individual 111
```

We could instead use the argument `alphatype = "varying"` to use the α that minimizes the CV MSE for each individual group:

```
preds = predict(cvfit, xtest, groupstest=groupstest, ytest=ytest,
                alphatype="varying")
preds
#>
#> Call:
#> predict.cv.ptLasso(cvfit = cvfit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest, alphatype = "varying")
#>
#>
#> alpha:
#> group_1 group_2 group_3 group_4 group_5
#>     0.5     0.4     0.3     0.7     0.2
#>
#>
#> Performance (Mean squared error):
#>            overall  mean wtdMean group_1 group_2 group_3 group_4 group_5
#> Overall      757.1 757.1   757.1   815.7   542.6   567.1   792.7  1067.5
#> Pretrain     485.3 485.3   485.3   490.7   439.0   517.1   520.3   459.5
#> Individual   529.3 529.3   529.3   572.6   441.8   562.4   550.5   518.9
#>
#>
#> Support size:
#>
#> Overall    50
#> Pretrain   94 (20 common + 74 individual)
#> Individual 111
```

4 Other details

4.1 Choosing α, the pretraining hyperparameter

Selecting the hyperparameter α is an important part of pretraining. The simplest way to do this is to use `cv.ptLasso` – this will automatically perform pretraining for a range of α values and return the CV performance for each. The default values for α are $0, 0.1, 0.2, \ldots, 1$.

```
cvfit <- cv.ptLasso(x, y, groups)
cvfit
#>
#> Call:
#> cv.ptLasso(x = x, y = y, groups = groups, family = "gaussian",
#>     type.measure = "mse", use.case = "inputGroups")
#>
#>
#>
#> type.measure:  mse
#>
#>
#>            alpha overall  mean wtdMean group_1 group_2 group_3 group_4 group_5
#> Overall            703.1 703.1   703.1   723.0   502.8   577.2   665.9  1046.6
#> Pretrain     0.0   559.7 559.7   559.7   460.2   504.7   611.5   539.7   682.6
#> Pretrain     0.1   504.2 504.2   504.2   434.7   464.5   575.8   488.3   557.6
#> Pretrain     0.2   499.7 499.7   499.7   401.6   448.5   610.8   494.5   543.0
#> Pretrain     0.3   487.1 487.1   487.1   387.9   449.2   588.2   479.7   530.7
#> Pretrain     0.4   491.0 491.0   491.0   401.6   465.2   571.5   471.3   545.3
#> Pretrain     0.5   489.3 489.3   489.3   368.4   452.6   586.5   481.1   558.1
#> Pretrain     0.6   501.6 501.6   501.6   376.8   473.0   587.8   491.5   579.1
#> Pretrain     0.7   506.8 506.8   506.8   391.8   466.5   617.2   490.6   567.7
#> Pretrain     0.8   513.9 513.9   513.9   415.6   477.9   604.4   468.2   603.6
#> Pretrain     0.9   509.8 509.8   509.8   383.0   485.4   601.3   504.0   575.3
#> Pretrain     1.0   527.5 527.5   527.5   393.4   478.8   639.2   510.2   615.7
#> Individual         527.5 527.5   527.5   393.4   478.8   639.2   510.2   615.7
#>
#> alphahat (fixed) = 0.3
#> alphahat (varying):
#> group_1 group_2 group_3 group_4 group_5
#>     0.5     0.2     0.4     0.8     0.3
```

Of course, you can specify the values of α to consider:

```
cvfit <- cv.ptLasso(x, y, groups, alphalist = c(0, 0.5, 1))
cvfit
#>
#> Call:
#> cv.ptLasso(x = x, y = y, groups = groups, alphalist = c(0, 0.5,
#>     1), family = "gaussian", type.measure = "mse", use.case = "inputGroups")
#>
#>
#>
#> type.measure:  mse
#>
#>
#>            alpha overall  mean wtdMean group_1 group_2 group_3 group_4 group_5
```

```
#> Overall            704.1 704.1   704.1   742.2   502.8   571.4   670.5  1033.7
#> Pretrain     0.0   555.7 555.7   555.7   463.8   519.8   608.3   566.6   620.1
#> Pretrain     0.5   503.9 503.9   503.9   387.5   492.1   594.2   485.2   560.2
#> Pretrain     1.0   531.5 531.5   531.5   397.7   516.3   631.4   530.0   582.0
#> Individual         531.5 531.5   531.5   397.7   516.3   631.4   530.0   582.0
#>
#> alphahat (fixed) = 0.5
#> alphahat (varying):
#> group_1 group_2 group_3 group_4 group_5
#>     0.5     0.5     0.5     0.5     0.5
```

At prediction time, `cv.ptLasso` uses the α that had the best CV performance on average across all groups. We could instead choose to use a different α for each group, as `cv.ptLasso` already figured out which α optimizes the CV performance for each group. To use group-specific values of α, specify `alphatype = "varying"` at prediction time. In this example, the best group-specific α values all happen to be 0.5 – the same as the overall α.

```
################################################
# Common alpha for all groups:
################################################
predict(cvfit, xtest, groupstest, ytest=ytest)
#>
#> Call:
#> predict.cv.ptLasso(cvfit = cvfit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
#> alpha =  0.5
#>
#> Performance (Mean squared error):
#>
#>            allGroups  mean group_1 group_2 group_3 group_4 group_5    r^2
#> Overall        757.1 757.1   815.7   542.6   567.1   792.7  1067.5 0.5362
#> Pretrain       498.1 498.1   549.4   431.0   532.5   501.5   475.8 0.6949
#> Individual     528.8 528.8   584.1   441.7   567.2   548.0   503.3 0.6760
#>
#> Support size:
#>
#> Overall    50
#> Pretrain   98 (20 common + 78 individual)
#> Individual 108

################################################
# Different alpha for each group:
################################################
predict(cvfit, xtest, groupstest, ytest=ytest, alphatype = "varying")
#>
#> Call:
#> predict.cv.ptLasso(cvfit = cvfit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest, alphatype = "varying")
#>
#>
#> alpha:
#> group_1 group_2 group_3 group_4 group_5
```

```
#>     0.5     0.5     0.5     0.5     0.5
#>
#>
#> Performance (Mean squared error):
#>            overall  mean wtdMean group_1 group_2 group_3 group_4 group_5
#> Overall      757.1 757.1   757.1   815.7   542.6   567.1   792.7  1067.5
#> Pretrain     498.1 498.1   498.1   549.4   431.0   532.5   501.5   475.8
#> Individual   528.8 528.8   528.8   584.1   441.7   567.2   548.0   503.3
#>
#>
#> Support size:
#>
#> Overall    50
#> Pretrain   98 (20 common + 78 individual)
#> Individual 108
```

4.2 Choosing λ, the lasso hyperparameter, for the first stage of pretraining

The first step of pretraining fits the overall model with `cv.glmnet` and selects a model along the λ path. The second stage uses the overall model's support and predictions to train the group-specific models.

So, at train time, we need to know choose a value of λ to use for the first stage. This can be specified in `ptLasso` with the argument `overall.lambda`. The default value of `overall.lambda` is "lambda.1se", as we found through simulations and real data examples that this usually had slightly better performance than the natural alternative, "lambda.min". But this is free for you to change: `overall.lambda` can accept "lambda.1se" or "lambda.min" (as in `predict.cv.glmnet`).

Whatever choice is made at train time will be automatically used at test time, and this cannot be changed. (The fitted model from the second stage of pretraining expects the offset to have been computed using a particular model – it does not make sense to compute the offset using a different model with a different λ!)

```
# Default:
fit <- ptLasso(x, y, groups, alpha = 0.5, overall.lambda = "lambda.1se")

# Alternative:
fit <- ptLasso(x, y, groups, alpha = 0.5, overall.lambda = "lambda.min")
```

4.3 Fitting elasticnet or ridge models

By default, `ptLasso` fits lasso penalized models; in `glmnet`, this corresponds to the elasticnet parameter $\alpha_{\text{en}} = 1$ (where the subscript `en` stands for "elasticnet"). Fitting pretrained elasticnet or ridge models is also possible with `ptLasso`: simply pass in the argument `en.alpha` between 0 (ridge) and 1 (lasso). Here is an example using the pretraining hyperparameter $\alpha = 0.5$ and the elasticnet hyperparameter `en.alpha = 0.2`.

```
fit <- ptLasso(x, y, groups,
               alpha = 0.5,    # pretraining hyperparameter
               en.alpha = 0.2) # elasticnet hyperparameter
```

4.4 Printing progress during model training

When models take a long time to train, it can be useful to print out progress during training. `ptLasso` has two ways to do this (and they can be combined). First, we can simply print out which model is being fitted using `verbose = TRUE`:

```
fit <- ptLasso(x, y, groups, alpha = 0.5, verbose = TRUE)
#> Fitting overall model
```

```
#> Fitting individual models
#>  Fitting individual model 1 / 5
#>  Fitting individual model 2 / 5
#>  Fitting individual model 3 / 5
#>  Fitting individual model 4 / 5
#>  Fitting individual model 5 / 5
#> Fitting pretrained lasso models
#>  Fitting pretrained model 1 / 5
#>  Fitting pretrained model 2 / 5
#>  Fitting pretrained model 3 / 5
#>  Fitting pretrained model 4 / 5
#>  Fitting pretrained model 5 / 5
```

We can also print out a progress bar for *each model* that is being fit – this functionality comes directly from `cv.glmnet`, and follows its notation. (To avoid cluttering this document, we do not run the following example.)

```
fit <- ptLasso(x, y, groups, alpha = 0.5, trace.it = TRUE)
```

And of course, we can combine these to print out (1) which model is being trained and (2) the corresponding progress bar.

```
fit <- ptLasso(x, y, groups, alpha = 0.5, verbose = TRUE, trace.it = TRUE)
```

4.5 Using individual and overall models that have already been trained

`ptLasso` will fit the overall and individual models. However, if you have already trained the overall or individual models, you can pass them directly to `ptLasso` and avoid refitting them. **`ptLasso` expects that these models were fitted using the same training data that you pass to `ptLasso`, and that they were fitted with the argument `keep = TRUE`.** Here is an example. We will fit an overall model and individual models, and then we will show how to pass them to `ptLasso`. Using `verbose = TRUE` in the call to `ptLasso` shows us what models are being trained (and confirms that we are not refitting the overall and individual models).

```
overall.model = cv.glmnet(x, y, keep = TRUE)
individual.models = lapply(1:5,
                           function(kk) cv.glmnet(x[groups == kk, ],
                                                  y[groups == kk],
                                                  keep = TRUE))

fit <- ptLasso(x, y, groups,
               fitoverall = overall.model,
               fitind = individual.models,
               verbose = TRUE)
#> Fitting pretrained lasso models
#>  Fitting pretrained model 1 / 5
#>  Fitting pretrained model 2 / 5
#>  Fitting pretrained model 3 / 5
#>  Fitting pretrained model 4 / 5
#>  Fitting pretrained model 5 / 5
```

Of course we could pass just the overall *or* individual models to ‘ptLasso:

```
fit <- ptLasso(x, y, groups, fitoverall = overall.model, verbose = TRUE)
#> Fitting individual models
#>  Fitting individual model 1 / 5
```

```
#>  Fitting individual model 2 / 5
#>  Fitting individual model 3 / 5
#>  Fitting individual model 4 / 5
#>  Fitting individual model 5 / 5
#> Fitting pretrained lasso models
#>  Fitting pretrained model 1 / 5
#>  Fitting pretrained model 2 / 5
#>  Fitting pretrained model 3 / 5
#>  Fitting pretrained model 4 / 5
#>  Fitting pretrained model 5 / 5
```

```
fit <- ptLasso(x, y, groups, fitind = individual.models, verbose = TRUE)
#> Fitting overall model
#> Fitting pretrained lasso models
#>  Fitting pretrained model 1 / 5
#>  Fitting pretrained model 2 / 5
#>  Fitting pretrained model 3 / 5
#>  Fitting pretrained model 4 / 5
#>  Fitting pretrained model 5 / 5
```

4.6 Fitting the overall model without group-specific intercepts

When we fit the overall model with input grouped data, we solve the following:

$$\hat{\mu_0}, \hat{\theta_2}, \ldots, \hat{\theta_K}, \hat{\beta}_0 = \arg\min_{\mu, \theta_2, \ldots, \theta_k, \beta} \frac{1}{2} \sum_{k=1}^{K} \|y_k - (\mu \mathbf{1} + \theta_k \mathbf{1} + X_k \beta)\|_2^2 + \lambda ||\beta||_1, \tag{5}$$

where $\hat{\theta_1}$ is defined to be 0. If we do not want a separate intercept for each group $(\theta_1, \ldots, \theta_K)$, we can instead fit the following:

$$\hat{\mu_0}, \hat{\beta}_0 = \arg\min_{\mu, \beta} \frac{1}{2} \sum_{k=1}^{K} \|y_k - (\mu \mathbf{1} + X_k \beta)\|_2^2 + \lambda ||\beta||_1. \tag{6}$$

This may be useful in settings where the groups are different between train and test sets and we show an example in the section "Different groups in train and test data". To do this, use the argument `group.intercepts = FALSE`. In our toy example, omitting the group-specific intercepts results in slightly worse CV performance; we expect this to be the case more generally.

```
cvfit <- cv.ptLasso(x, y, groups, group.intercepts = FALSE)
cvfit
#>
#> Call:
#> cv.ptLasso(x = x, y = y, groups = groups, group.intercepts = FALSE,
#>     family = "gaussian", type.measure = "mse", use.case = "inputGroups")
#>
#>
#>
#> type.measure:  mse
#>
#>
#>            alpha overall  mean wtdMean group_1 group_2 group_3 group_4 group_5
#> Overall            694.2 694.2   694.2   716.0   503.8   580.4   667.5  1003.3
#> Pretrain     0.0   583.9 583.9   583.9   522.0   496.7   591.8   597.9   711.1
#> Pretrain     0.1   523.0 523.0   523.0   435.2   486.0   587.2   480.3   626.2
#> Pretrain     0.2   524.3 524.3   524.3   430.6   453.5   629.6   496.6   611.3
```

```
#> Pretrain     0.3   526.0 526.0   526.0   418.7   466.9   617.5   530.9   596.1
#> Pretrain     0.4   514.1 514.1   514.1   390.5   474.4   574.9   504.7   626.0
#> Pretrain     0.5   515.7 515.7   515.7   379.9   484.3   590.5   528.5   595.2
#> Pretrain     0.6   509.9 509.9   509.9   385.5   467.0   600.7   484.7   611.6
#> Pretrain     0.7   507.0 507.0   507.0   392.8   478.2   590.3   488.1   585.3
#> Pretrain     0.8   507.5 507.5   507.5   382.0   478.5   593.9   490.6   592.4
#> Pretrain     0.9   526.6 526.6   526.6   409.6   486.9   634.3   510.5   591.9
#> Pretrain     1.0   509.3 509.3   509.3   397.7   501.6   599.7   474.1   573.3
#> Individual         509.3 509.3   509.3   397.7   501.6   599.7   474.1   573.3
#>
#> alphahat (fixed) = 0.7
#> alphahat (varying):
#> group_1 group_2 group_3 group_4 group_5
#>     0.5     0.2     0.4     1.0     1.0
```

4.7 Arguments for use in `cv.glmnet`

Because model fitting is done with `cv.glmnet`, `ptLasso` can take and pass arguments to `glmnet`. Notable choices include `penalty.factor`, `weights`, `upper.limits`, `lower.limits` and `en.alpha` (known as `alpha` in `glmnet`). Please refer to the `glmnet` documentation for more information on their use.

`ptLasso` does not support the arguments `intercept`, `offset`, `fit` and `check.args`.

4.8 Parallelizing model fitting

For large datasets, we can parallelize model fitting within the calls to `cv.glmnet`. As in `cv.glmnet`, pass the argument `parallel = TRUE`, and register parallel beforehand:

```
require(doMC)
registerDoMC(cores = 4)
fit = ptLasso(x, y, groups = groups, family = "gaussian", type.measure = "mse",
              parallel=TRUE)
```

5 Input grouped data

5.1 Base case: input grouped data with a binomial outcome

In the Quick Start, we applied `ptLasso` to data with a continuous response. Here, we'll use data with a binary outcome. This creates a dataset with $k = 3$ groups (each with 100 observations), 5 shared coefficients, and 5 coefficients specific to each group.

```
set.seed(1234)

out = binomial.example.data()
x = out$x; y = out$y; groups = out$groups

outtest = binomial.example.data()
xtest = outtest$x; ytest = outtest$y; groupstest = outtest$groups
```

We can fit and predict as before. By default, `predict.ptLasso` will compute and return the *deviance* on the test set.

```
fit = ptLasso(x, y, groups, alpha = 0.5, family = "binomial")

predict(fit, xtest, groupstest, ytest = ytest)
```

```
#>
#> Call:
#> predict.ptLasso(fit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
#> alpha =  0.5
#>
#> Performance (Deviance):
#>
#>            allGroups  mean wtdMean group_1 group_2 group_3
#> Overall        1.360 1.360   1.360   1.340   1.334   1.405
#> Pretrain       1.277 1.277   1.277   1.211   1.224   1.396
#> Individual     1.279 1.279   1.279   1.252   1.186   1.399
#>
#> Support size:
#>
#> Overall    3
#> Pretrain   12 (3 common + 9 individual)
#> Individual 14
```

We could instead compute the AUC by specifying the `type.measure` in the call to `ptLasso`. Note: `type.measure` is specified during model fitting and not prediction because it is used in each call to `cv.glmnet`.

```
fit = ptLasso(x, y, groups, alpha = 0.5, family = "binomial",
              type.measure = "auc")
#> Warning: from glmnet C++ code (error code -99); Convergence for 99th lambda
#> value not reached after maxit=100000 iterations; solutions for larger lambdas
#> returned
#> Warning: from glmnet C++ code (error code -98); Convergence for 98th lambda
#> value not reached after maxit=100000 iterations; solutions for larger lambdas
#> returned

predict(fit, xtest, groupstest, ytest = ytest)
#>
#> Call:
#> predict.ptLasso(fit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
#> alpha =  0.5
#>
#> Performance (AUC):
#>
#>            allGroups   mean wtdMean group_1 group_2 group_3
#> Overall       0.6022 0.6009  0.6009  0.5957  0.6680  0.5390
#> Pretrain      0.6419 0.6707  0.6707  0.7169  0.7772  0.5182
#> Individual    0.6285 0.6576  0.6576  0.6805  0.7732  0.5190
#>
#> Support size:
#>
#> Overall    3
#> Pretrain   39 (2 common + 37 individual)
#> Individual 39
```

To fit the overall and individual models, we can use elasticnet instead of lasso by defining the parameter `en.alpha`. (as in `glmnet` and described in the section "Fitting elasticnet or ridge models").

```
fit = ptLasso(x, y, groups, alpha = 0.5, family = "binomial",
              type.measure = "auc",
              en.alpha = .5)
predict(fit, xtest, groupstest, ytest = ytest)
#>
#> Call:
#> predict.ptLasso(fit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
#> alpha =  0.5
#>
#> Performance (AUC):
#>
#>            allGroups   mean wtdMean group_1 group_2 group_3
#> Overall       0.6071 0.6087  0.6087  0.6365  0.6845  0.5051
#> Pretrain      0.6381 0.6525  0.6525  0.7226  0.7210  0.5141
#> Individual    0.6676 0.6702  0.6702  0.7013  0.7672  0.5422
#>
#> Support size:
#>
#> Overall    20
#> Pretrain   39 (3 common + 36 individual)
#> Individual 28
```

Using cross validation is the same as in the Gaussian case:

```
####################################################
# Fit:
####################################################
fit = cv.ptLasso(x, y, groups, family = "binomial", type.measure = "auc")
#> Warning: from glmnet C++ code (error code -89); Convergence for 89th lambda
#> value not reached after maxit=100000 iterations; solutions for larger lambdas
#> returned
#> Warning: from glmnet C++ code (error code -91); Convergence for 91th lambda
#> value not reached after maxit=100000 iterations; solutions for larger lambdas
#> returned
#> Warning: from glmnet C++ code (error code -87); Convergence for 87th lambda
#> value not reached after maxit=100000 iterations; solutions for larger lambdas
#> returned

####################################################
# Predict with a common alpha for all groups:
####################################################
predict(fit, xtest, groupstest, ytest = ytest)
#>
#> Call:
#> predict.cv.ptLasso(cvfit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
#> alpha =  0.4
```

```
#>
#> Performance (AUC):
#>
#>            allGroups   mean wtdMean group_1 group_2 group_3
#> Overall       0.6070 0.6072  0.6072  0.5985  0.6764  0.5467
#> Pretrain      0.6289 0.6561  0.6561  0.6809  0.7700  0.5173
#> Individual    0.6409 0.6567  0.6567  0.6728  0.7732  0.5241
#>
#> Support size:
#>
#> Overall    3
#> Pretrain   39 (2 common + 37 individual)
#> Individual 40

##################################################
# Predict with a different alpha for each group:
##################################################
predict(fit, xtest, groupstest, ytest = ytest, alphatype = "varying")
#>
#> Call:
#> predict.cv.ptLasso(cvfit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest, alphatype = "varying")
#>
#>
#> alpha:
#> group_1 group_2 group_3
#>     0.9     0.8     0.4
#>
#>
#> Performance (AUC):
#>            overall   mean wtdMean group_1 group_2 group_3
#> Overall     0.6070 0.6072  0.6072  0.5985  0.6764  0.5467
#> Pretrain    0.6359 0.6520  0.6520  0.6752  0.7635  0.5173
#> Individual  0.6409 0.6567  0.6567  0.6728  0.7732  0.5241
#>
#>
#> Support size:
#>
#> Overall    3
#> Pretrain   39 (2 common + 37 individual)
#> Individual 40
```

5.2 Base case: input grouped survival data

```
require(survival)
#> Loading required package: survival
```

Now, we will simulate survival times with 3 groups; the three groups have overlapping support, with 5 shared features and each has 5 individual features. To compute survival time, we start by computing survival $= X\beta + \epsilon$, where β is specific to each group and ϵ is noise. Because survival times must be positive, we modify this to be survival $=$ survival $+ 1.1 *$ abs(min(survival)).

```r
set.seed(1234)

n = 600; ntrain = 300
p = 50

x = matrix(rnorm(n*p), n, p)
beta1 = c(rnorm(5), rep(0, p-5))

beta2 = runif(p) * beta1 # Shared support
beta2 = beta2 + c(rep(0, 5), rnorm(5), rep(0, p-10)) # Individual features

beta3 = runif(p) * beta1 # Shared support
beta3 = beta3 + c(rep(0, 10), rnorm(5), rep(0, p-15)) # Individual features

# Randomly split into groups
groups = sample(1:3, n, replace = TRUE)

# Compute survival times:
survival = x %*% beta1
survival[groups == 2] = x[groups == 2, ] %*% beta2
survival[groups == 3] = x[groups == 3, ] %*% beta3
survival = survival + rnorm(n)
survival = survival + 1.1 * abs(min(survival))

# Censoring times from a random uniform distribution:
censoring = runif(n, min = 1, max = 10)

# Did we observe surivival or censoring?
y = Surv(pmin(survival, censoring), survival <= censoring)

# Split into train and test:
xtest = x[-(1:300), ]
ytest = y[-(1:300), ]
groupstest = groups[-(1:300)]

x = x[1:300, ]
y = y[1:300, ]
groups = groups[1:300]
```

Training with `ptLasso` is much the same as it was for the continuous and binomial cases; the only difference is that we specify `family = "cox"`. By default, `ptLasso` uses the partial likelihood for model selection. We could instead use the C index.

```r
############################################################
# Default -- use partial likelihood as the type.measure:
############################################################
fit = ptLasso(x, y, groups, alpha = 0.5, family = "cox")
predict(fit, xtest, groupstest, ytest = ytest)
#>
#> Call:
#> predict.ptLasso(fit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
```

```
#> alpha =  0.5
#>
#> Performance (Deviance):
#>
#>            allGroups   mean wtdMean group_1 group_2 group_3
#> Overall        382.4  88.05   89.75   100.3  106.24   57.56
#> Pretrain       404.8  92.08   92.95   112.2   98.03   65.98
#> Individual     514.1 111.28  112.13   116.4  120.60   96.83
#>
#> Support size:
#>
#> Overall    8
#> Pretrain   33 (5 common + 28 individual)
#> Individual 33

############################################################
# Alternatively -- use the C index:
############################################################
fit = ptLasso(x, y, groups, alpha = 0.5, family = "cox", type.measure = "C")
predict(fit, xtest, groupstest, ytest = ytest)
#>
#> Call:
#> predict.ptLasso(fit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
#> alpha =  0.5
#>
#> Performance (C-index):
#>
#>            allGroups   mean wtdMean group_1 group_2 group_3
#> Overall       0.8427 0.8569  0.8495  0.8997  0.7544  0.9164
#> Pretrain      0.8101 0.8197  0.8215  0.9087  0.8197  0.7307
#> Individual    0.7974 0.7969  0.7994  0.8972  0.8031  0.6904
#>
#> Support size:
#>
#> Overall    18
#> Pretrain   37 (5 common + 32 individual)
#> Individual 39
```

The call to `cv.ptLasso` is again much the same; we only need to specify `family` ("cox") and `type.measure` (if we want to use the C index instead of the partial likelihood).

```
####################################################
# Fit:
####################################################
fit = cv.ptLasso(x, y, groups, family = "cox", type.measure = "C")

####################################################
# Predict with a common alpha for all groups:
####################################################
predict(fit, xtest, groupstest, ytest = ytest)
#>
```

```
#> Call:
#> predict.cv.ptLasso(cvfit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest)
#>
#>
#> alpha =  0.5
#>
#> Performance (C-index):
#>
#>            allGroups   mean wtdMean group_1 group_2 group_3
#> Overall       0.8527 0.8652  0.8586  0.9113  0.7711  0.9133
#> Pretrain      0.8606 0.8565  0.8550  0.9177  0.8221  0.8297
#> Individual    0.7642 0.8088  0.8128  0.9126  0.8327  0.6811
#>
#> Support size:
#>
#> Overall    8
#> Pretrain   23 (4 common + 19 individual)
#> Individual 27

####################################################
# Predict with a different alpha for each group:
####################################################
predict(fit, xtest, groupstest, ytest = ytest, alphatype = "varying")
#>
#> Call:
#> predict.cv.ptLasso(cvfit = fit, xtest = xtest, groupstest = groupstest,
#>     ytest = ytest, alphatype = "varying")
#>
#>
#> alpha:
#> group_1 group_2 group_3
#>     0.6     0.7     0.2
#>
#>
#> Performance (C-index):
#>            overall   mean wtdMean group_1 group_2 group_3
#> Overall     0.8527 0.8652  0.8586  0.9113  0.7711  0.9133
#> Pretrain    0.7969 0.8457  0.8457  0.9165  0.8280  0.7926
#> Individual  0.7642 0.8088  0.8128  0.9126  0.8327  0.6811
#>
#>
#> Support size:
#>
#> Overall    8
#> Pretrain   25 (4 common + 21 individual)
#> Individual 27
```

5.3 Different groups in train and test data

Suppose we observe groups at test time that were unobserved at train time. For example, our training set may consist of K *people* – each with many observations – and at test time, we wish to make predictions for observations from new people. We can still use pretraining in this setting: train a model using all data, and use this to guide the training for person-specific models.

Now however, we also fit an extra model to predict the similarity of test observations to the observations from each of the *training people*. To train this model, we use the (training) observation matrix X and the response y_{sim}, where $y_{\text{sim}} = k$ for all observations from the k^{th} person. When used for prediction, this model gives us a similarity (or probability) vector of length K that sums to 1, describing how similar an observation is to each training person.

At test time, we make predictions from (1) each pretrained person-specific model and (2) the person-similarity model, and we compute the weighted average of the pretrained predictions with respect to the similarity vector. Here is an example using simulated data.

```
set.seed(1234)

# Start with 5 people, each with 300 observations and 200 features.
# 3 people will be used for training, and 2 for testing.
n = 300*5; p = 200;
groups = sort(rep(1:5, n/5))

# We will have different coefficients for each of the 3 training people,
# and the first 3 features are shared support.
beta.group1 = c(-1, 1, 1, rep(0.5, 3), rep(0, p-6));
beta.group2 = c(-1, 1, 1, rep(0, 3), rep(0.5, 3), rep(0, p-9));
beta.group3 = c(-1, 1, 1, rep(0, 6), rep(0.5, 3), rep(0, p-12));

# The two test people are each a combination of of the training people.
# Person 4 will have observations drawn from classes 1 and 2, and
# Person 5 will have observations drawn from classes 1 and 3.
# The vector "hidden groups" is a latent variable - used to simulate data
# but unobserved in real data.
hidden.gps = groups
hidden.gps[hidden.gps == 4] = sample(c(1, 2), sum(groups == 4), replace = TRUE)
hidden.gps[hidden.gps == 5] = sample(c(1, 3), sum(groups == 5), replace = TRUE)

# We modify X according to group membership;
# we want X to cluster into groups 1, 2 and 3.
x = matrix(rnorm(n * p), nrow = n, ncol = p)
x[hidden.gps == 1, 1:3] = x[hidden.gps == 1, 1:3] + 1
x[hidden.gps == 2, 1:3] = x[hidden.gps == 2, 1:3] + 2
x[hidden.gps == 3, 1:3] = x[hidden.gps == 3, 1:3] + 3

# And now, we compute y using betas 1, 2 and 3:
x.beta = rep(0, n)
x.beta[hidden.gps == 1] = x[hidden.gps == 1, ] %*% beta.group1
x.beta[hidden.gps == 2] = x[hidden.gps == 2, ] %*% beta.group2
x.beta[hidden.gps == 3] = x[hidden.gps == 3, ] %*% beta.group3
y = x.beta + 5 * rnorm(n)
```

We're ready to split into train, validation and test sets. We will use people 1, 2 and 3 for training and validation (two-thirds train, one-third validation), and people 4 and 5 for testing.

```
trn.index = groups < 4
val.sample = sample(1:sum(trn.index), 1/3 * sum(trn.index), replace = FALSE)

xtrain = x[trn.index, ][-val.sample, ]
ytrain = y[trn.index][-val.sample]
gpstrain = groups[trn.index][-val.sample]
```

```
xval   = x[trn.index, ][val.sample, ]
yval = y[trn.index][val.sample]
gpsval = groups[trn.index][val.sample]

xtest  = x[!trn.index, ]
ytest = y[!trn.index]
gpstest = groups[!trn.index]
```

We start with pretraining, where the person ID is the grouping variable.

```
cvfit = cv.ptLasso(xtrain, ytrain, gpstrain,
                   type.measure = "mse",
                   group.intercepts = FALSE,
                   overall.lambda = "lambda.1se")
```

Now, we train a model to predict the person ID from the covariates. Because this example is simulated, we can measure the performance of our model on test data (via the confusion matrix comparing predicted group labels to true labels). In real settings, this would be impossible.

```
simmod = cv.glmnet(xtrain, as.factor(gpstrain), family = "multinomial")

# Peek at performance on test data.
# Not possible with real data.
class.preds = predict(simmod, xtest, type="response")[, , 1]
table(apply(class.preds, 1, which.max),
      hidden.gps[groups >= 4])
#>
#>       1   2   3
#>   1 259  35   3
#>   2  40  85  27
#>   3   0  35 116
```

Finally we can make predictions: we have everything we need. For each test observation, we will get the pretrained prediction for all 3 training classes. Our final predictions are the weighted combination of the predictions from `ptLasso` and the class predictions from `glmnet`.

```
alphahat  = cvfit$alphahat
bestmodel = cvfit$fit[[which(cvfit$alphalist == alphahat)]]
cat("Chosen alpha is", alphahat, ".\n")
#> Chosen alpha is 0.5 .

offset = (1-alphahat) * predict(bestmodel$fitoverall, xtest, s = "lambda.1se")

# Get the prediction for all three classes for each test observation.
# This will be a matrix with three columns; one for each class.
pretrained.preds = do.call(cbind,
                           lapply(1:3,
                                  function(i) predict(bestmodel$fitpre[[i]],
                                                      xtest,
                                                      newoffset = offset)
                           )
)

assess.glmnet( rowSums(pretrained.preds * class.preds), newy = ytest)$mse
#> [1] 28.68004
#> attr(,"measure")
```

```
#> [1] "Mean-Squared Error"
```

There are two reasonable baselines. The first is the overall model with no grouping at all, and the second is the set of individual models (one for each group).

```
##########################################################
# Baseline 1: overall model
##########################################################
overall.predictions = predict(cvfit$fitoverall, xtest)
assess.glmnet(overall.predictions, newy = ytest)$mse
#> lambda.1se
#>   29.64747
#> attr(,"measure")
#> [1] "Mean-Squared Error"

##########################################################
# Baseline 2: individual models
##########################################################
individual.preds = do.call(cbind,
                           lapply(1:3,
                                  function(i) predict(bestmodel$fitind[[i]],
                                                      xtest,
                                                      type = "response")
                           )
)
assess.glmnet(rowSums(individual.preds * class.preds), newy = ytest)$mse
#> [1] 28.87445
#> attr(,"measure")
#> [1] "Mean-Squared Error"
```

What we have done – taking a weighted average of predictions with respect to similarity to each person – makes sense mathematically. However, we have found better empirical results if we instead train a supervised learning algorithm to make the final prediction $\hat{y}$ using the pretrained model predictions and the class similarity predictions as features. So, let's do that here, using our so-far-untouched validation set.

```
val.offset = predict(bestmodel$fitoverall, xval, s = "lambda.1se")
val.offset = (1 - alphahat) * val.offset
val.preds = do.call(cbind,
                    lapply(1:3, function(i) predict(bestmodel$fitpre[[i]],
                                                    xval,
                                                    newoffset = val.offset,
                                                    type = "response")
                    )
)
val.class.preds = predict(simmod, xval)[, , 1]

pred.data = cbind(val.preds, val.class.preds, val.preds * val.class.preds)
final.model = cv.glmnet(pred.data, rowSums(val.preds * val.class.preds))

pred.data.test = cbind(pretrained.preds,
                       class.preds,
                       pretrained.preds * class.preds)
assess.glmnet(predict(final.model, pred.data.test), newy = ytest)$mse
#> lambda.1se
#>   28.84557
```

```
#> attr(,"measure")
#> [1] "Mean-Squared Error"
```

Comparing performance of all models side-by-side shows that (1) using input groups improved performance – including for the individual models and (2) including the final model did not help performance (but we still recommend trying this with real data).

```
rd = function(x) round(x, 2)

cat("Overall model PSE: ",
    rd(assess.glmnet(overall.predictions, newy = ytest)$mse))
#> Overall model PSE:  29.65

cat("Individual model PSE: ",
    rd(assess.glmnet(rowSums(individual.preds*class.preds), newy = ytest)$mse))
#> Individual model PSE:  28.87

cat("Pretraining model PSE: ",
    rd(assess.glmnet(rowSums(pretrained.preds*class.preds), newy = ytest)$mse))
#> Pretraining model PSE:  28.68

cat("Pretraining model + final prediction model PSE: ",
    rd(assess.glmnet(predict(final.model,
                             cbind(pretrained.preds,
                                   class.preds,
                                   pretrained.preds * class.preds)
                         ),
                 newy = ytest)$mse))
#> Pretraining model + final prediction model PSE:  28.85
```

5.4 Learning the input groups

Suppose we have a dataset with features X and response y, and no input grouping. Suppose we also have a small set of meaningful features Z that we expect to stratify observations (e.g. in biomedicine, Z may consist of age and sex). In this setting, we can *learn* input groups using Z.

The steps to do this are as follows.

1. Partition data into two sets: one to learn the grouping and one to do pretraining.
2. With the first set, train a small CART tree using Z and y.
3. Make predictions for the remaining data; assign observations to groups according to their terminal nodes.
4. Apply pretraining using the learned group assignments.

Here, we show an example using simulated data. We use `rpart` to train a CART tree. The package `ODRF` (Liu and Xia (2022)) is another good choice – it fits a linear model in each terminal node, which is closer to what pretraining does, and may therefore have better performance.

```
require(rpart)
#> Loading required package: rpart
```

Simulate data with a binary outcome: X is drawn from a random normal (with $p = 50$ uncorrelated features), and Z is simulated as age (uniform between 20 and 90) and sex (half 0, half 1). The *true* groups are (1) age under 50, (2) age over 50 and sex = 0 and (3) age over 50 and sex = 1.

```
set.seed(1234)
```

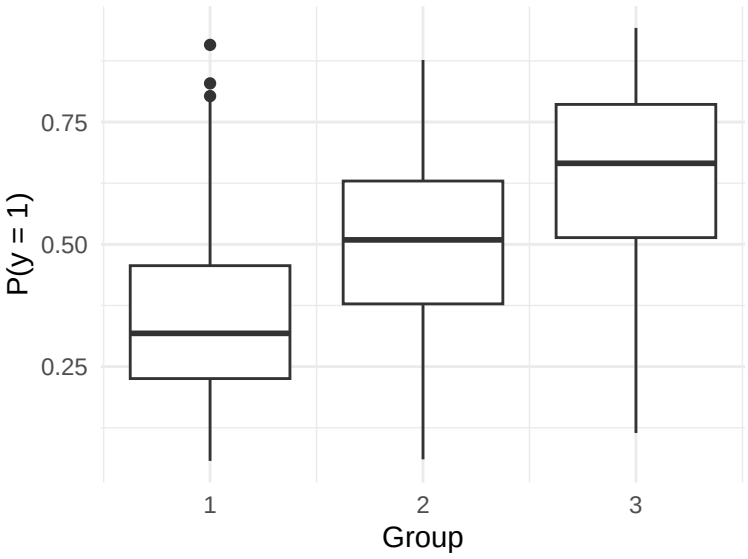
```
n = 1000; p = 50
groupvars = cbind(age = round(runif(n, min = 20, max = 90)),
                  sex = sample(c(0, 1), n, replace = TRUE))
groups = rep(1, n)
groups[groupvars[, "age"] > 50 & groupvars[, "sex"] == 0] = 2
groups[groupvars[, "age"] > 50 & groupvars[, "sex"] == 1] = 3
```

Now, we'll define coefficients β_k such that $P(y_i = 1 \mid x_i) = \frac{1}{1+\exp(-x_i^T \beta_k)}$ for each group. Across groups, three coefficients are shared, three are group-specific and the rest are 0. Each group has a unique intercept to adjust its baseline risk.

```
beta.group1 = c(-0.5, 0.5, 0.1, c(0.1, 0.2, 0.3), rep(0, p-6));
beta.group2 = c(-0.5, 0.5, 0.1, rep(0, 3), c(0.1, 0.2, 0.3), rep(0, p-9));
beta.group3 = c(-0.5, 0.5, 0.1, rep(0, 6), c(0.1, 0.2, 0.3), rep(0, p-12));

x = matrix(rnorm(n * p), nrow = n, ncol = p)
x.beta = rep(0, n)
x.beta[groups == 1] = x[groups == 1, ] %*% beta.group1 - 0.75
x.beta[groups == 2] = x[groups == 2, ] %*% beta.group2
x.beta[groups == 3] = x[groups == 3, ] %*% beta.group3 + 0.75

y = rbinom(n, size = 1, prob = 1/(1 + exp(-x.beta)))

# Now that we have our data, we will partition it into 3 datasets:
# one to cluster, one to train models and one to test performance.
xcluster = x[1:250, ]; xtrain = x[251:750, ]; xtest = x[751:1000, ];
ycluster = y[1:250];   ytrain = y[251:750];   ytest = y[751:1000];

zcluster = groupvars[1:250, ];
ztrain = groupvars[251:750, ];
ztest = groupvars[751:1000, ];

# We will use this just to see how our clustering performed.
# Not possible with real data!
groupstrain = groups[251:750];
```

By design, $P(y = 1)$ is different across groups:

```
ggplot() +
  geom_boxplot(aes(x=groups, y=1/(1 + exp(-x.beta)), group = groups)) +
  labs(x = "Group", y = "P(y = 1)") +
  theme_minimal()
```



We cluster using `rpart`. Note that we use `maxdepth = 2`: an obvious choice because we simulated the data and we know that there is a second-level interaction (age + sex) that determines outcome. In general, however, we recommend keeping this tree small (`maxdepth` smaller than 4) so that it is easily interpretable.

```
treefit = rpart(ycluster~.,
                data = data.frame(zcluster, ycluster),
                control=rpart.control(maxdepth=2, minbucket=20))
treefit
#> n= 250
#>
#> node), split, n, deviance, yval
#>       * denotes terminal node
#>
#> 1) root 250 61.82400 0.4480000
#>   2) age< 50.5 111 23.18919 0.2972973 *
#>   3) age>=50.5 139 34.10072 0.5683453
#>     6) sex< 0.5 56 13.92857 0.4642857 *
#>     7) sex>=0.5 83 19.15663 0.6385542 *
```

We want our tree to return the ID of the terminal node for each observation instead of class probabilities. The following is a trick that causes `predict` to behave as desired.

```
leaf=treefit$frame[,1]=="<leaf>"
treefit$frame[leaf,"yval"]=1:sum(leaf)

predgroupstrain = predict(treefit, data.frame(ztrain))
predgroupstest  = predict(treefit, data.frame(ztest))
```

Finally, we are ready to apply pretraining using the predicted groups as our grouping variable.

```
cvfit = cv.ptLasso(xtrain, ytrain, predgroupstrain, family = "binomial",
                   type.measure = "auc", nfolds = 10,
                   overall.lambda = "lambda.min")
predict(cvfit, xtest, predgroupstest, ytest = ytest)
#>
#> Call:
#> predict.cv.ptLasso(cvfit = cvfit, xtest = xtest, groupstest = predgroupstest,
#>     ytest = ytest)
```

```
#>
#>
#> alpha =  0.1
#>
#> Performance (AUC):
#>
#>            allGroups   mean wtdMean group_1 group_2 group_3
#> Overall       0.7068 0.6411  0.6362  0.6052  0.6556  0.6625
#> Pretrain      0.7212 0.6620  0.6531  0.6024  0.7006  0.6829
#> Individual    0.7004 0.6478  0.6402  0.5827  0.6428  0.7179
#>
#> Support size:
#>
#> Overall    11
#> Pretrain   21 (11 common + 10 individual)
#> Individual 6
```

Note that the overall model trained by `cv.ptLasso` takes advantage of the clustering: it fits a unique intercept for each group. Performance would have been much worse if we hadn't done any clustering at all:

```
baseline.model = cv.glmnet(xtrain, ytrain, family = "binomial", type.measure = "auc", nfolds = 5)
assess.glmnet(baseline.model, newx=xtest, newy=ytest)$auc
#> [1] 0.6050242
#> attr(,"measure")
#> [1] "AUC"
```

6 Target grouped data

Now we turn to the **target grouped** setting. Suppose we have a dataset with a multinomial outcome, and no other grouping on the observations. For example, our data might look like the following:

```
set.seed(1234)

n = 500; p = 75; k = 3
X = matrix(rnorm(n * p), nrow = n, ncol = p)
y = sample(1:k, n, replace = TRUE)

Xtest = matrix(rnorm(n * p), nrow = n, ncol = p)
```

Each row in X belongs to class 1, 2 or 3, and we wish to predict class membership. We could fit a single multinomial model to the data:

```
multinomial = cv.glmnet(X, y, family = "multinomial")

multipreds  = predict(multinomial, Xtest, s = "lambda.min")
multipreds.class = apply(multipreds, 1, which.max)
```

Or, we could fit 3 one-vs-rest models; at prediction time, we would assign observations to the class with the highest probability.

```
class1 = cv.glmnet(X, y == 1, family = "binomial")
class2 = cv.glmnet(X, y == 2, family = "binomial")
class3 = cv.glmnet(X, y == 3, family = "binomial")

ovrpreds = cbind(
  predict(class1, Xtest, s = "lambda.min"),
```

```
  predict(class2, Xtest, s = "lambda.min"),
  predict(class3, Xtest, s = "lambda.min"))
ovrpreds.class = apply(ovrpreds, 1, which.max)
```

Another alternative is to do pretraining, which fits something *in between* one model for all data and three separate models. `ptLasso` will do this for you, using the arguments `family = "multinomial"` and `use.case = "targetGroups"`.

```
fit = ptLasso(X, y, groups = y, alpha = 0.5,
              family = "multinomial", use.case = "targetGroups")
```

But what exactly is pretraining doing here? We'll walk through an example, doing pretraining "by hand". The steps are:

1. Train an overall model: a multinomial model using a penalty on the coefficients β so that each coefficient is either 0 or nonzero for all classes.
2. Train individual one-vs-rest models using the penalty factor and offset defined by the overall model (as in the input grouped setting).

To train the overall model, we use `cv.glmnet` with `type.multinomial = "grouped"`. This puts a penalty on β to force coefficients to be *in* or *out* of the model for all classes. This is analogous to the overall model in the input grouped setting: we want to first learn **shared** information.

```
multinomial = cv.glmnet(X, y, family = "multinomial",
                        type.multinomial = "grouped",
                        keep = TRUE)
```

Then, we fit 3 one-vs-rest models using the support and offset from the multinomial model.

```
# The support of the overall model:
nonzero.coefs = which((coef(multinomial, s = "lambda.1se")[[1]] != 0)[-1])

# The offsets - one for each class:
offset = predict(multinomial, X, s = "lambda.1se")
offset.class1 = offset[, 1, 1]
offset.class2 = offset[, 2, 1]
offset.class3 = offset[, 3, 1]
```

Now we have everything we need to train the one-vs-rest models. As always, we have the pretraining parameter α - for this example, let's use $\alpha = 0.5$:

```
alpha = 0.5
penalty.factor = rep(1/alpha, p)
penalty.factor[nonzero.coefs] = 1

class1 = cv.glmnet(X, y == 1, family = "binomial",
                   offset = (1-alpha) * offset.class1,
                   penalty.factor = penalty.factor)
class2 = cv.glmnet(X, y == 2, family = "binomial",
                   offset = (1-alpha) * offset.class2,
                   penalty.factor = penalty.factor)
class3 = cv.glmnet(X, y == 3, family = "binomial",
                   offset = (1-alpha) * offset.class3,
                   penalty.factor = penalty.factor)
```

And we're done with pretraining! To predict, we again assign each row to the class with the highest prediction:

Table 2: Coefficients for simulating target grouped data

	1-3	4-8	9-13	14-18	19-23	23-27	27-75
group 1	-0.2	-0.1	0.00	0	0.00	0.0	0
group 2	-0.1	0.0	-0.05	0	0.00	0.0	0
group 3	0.0	0.0	0.00	0	0.00	0.0	0
group 4	0.1	0.0	0.00	0	0.05	0.0	0
group 5	0.2	0.0	0.00	0	0.00	0.1	0

```
newoffset = predict(multinomial, X, s = "lambda.1se")
ovrpreds = cbind(
  predict(class1, Xtest, s = "lambda.min", newoffset = newoffset[, 1, 1]),
  predict(class2, Xtest, s = "lambda.min", newoffset = newoffset[, 2, 1]),
  predict(class3, Xtest, s = "lambda.min", newoffset = newoffset[, 3, 1])
)
ovrpreds.class = apply(ovrpreds, 1, which.max)
```

This is all done automatically within `ptLasso`; we show a more detailed example in the next section. The example above is intended only to show how pretraining works for multinomial outcomes, and some technical details have been omitted. (For example, `ptLasso` takes care of crossfitting between the first and second steps.)

6.1 Base case: data with a multinomial outcome

We will use `ptLasso` for data with a multinomial outcome. First, let's simulate multinomial data with 5 classes. We start by drawing X from a normal distribution (uncorrelated features), and then we shift the columns according to Table 2.

```
set.seed(1234)

n = 500; p = 75; k = 5
class.sizes = rep(n/k, k)
ncommon = 3; nindiv = 5;
shift.common = seq(-.2, .2, length.out = k)
shift.indiv  = seq(-.1, .1, length.out = k)

x     = matrix(rnorm(n * p), n, p)
xtest = matrix(rnorm(n * p), n, p)
y = ytest = c(sapply(1:length(class.sizes), function(i) rep(i, class.sizes[i])))

start = ncommon + 1
for (i in 1:k) {
  end = start + nindiv - 1
  x[y == i, 1:ncommon] = x[y == i, 1:ncommon] + shift.common[i]
  x[y == i, start:end] = x[y == i, start:end] + shift.indiv[i]

  xtest[ytest == i, 1:ncommon] = xtest[ytest == i, 1:ncommon] + shift.common[i]
  xtest[ytest == i, start:end] = xtest[ytest == i, start:end] + shift.indiv[i]
  start = end + 1
}
```

The calls to `ptLasso` and `cv.ptLasso` are almost the same as in the input grouped setting, only now we specify `use.case = "targetGroups"`. Note also that we use `groups = y`. The call to `predict` does not

require a `groups` argument because the groups are unknown at prediction time.

```
###############################################################################
# Fit the pretrained model.
# By default, ptLasso uses type.measure = "deviance", but for ease of
# interpretability, we use type.measure = "class" (the misclassification rate).
###############################################################################
fit = ptLasso(x = x, y = y, groups = y, family = "multinomial",
              use.case = "targetGroups", type.measure = "class")

###############################################################################
# Predict
###############################################################################
predict(fit, xtest, ytest = ytest)
#>
#> Call:
#> predict.ptLasso(fit = fit, xtest = xtest, ytest = ytest)
#>
#>
#>
#> alpha =  0.5
#>
#> Performance (Misclassification error):
#>
#>            overall   mean group_1 group_2 group_3 group_4 group_5
#> Overall      0.772
#> Pretrain     0.780 0.2000     0.2     0.2     0.2     0.2   0.200
#> Individual   0.788 0.1992     0.2     0.2     0.2     0.2   0.196
#>
#> Support size:
#>
#> Overall    52
#> Pretrain   37 (37 common + 0 individual)
#> Individual 37

###############################################################################
# Fit with CV to choose the alpha parameter
###############################################################################
cvfit = cv.ptLasso(x = x, y = y, groups = y, family = "multinomial",
              use.case = "targetGroups", type.measure = "class")

###############################################################################
# Predict using one alpha for all classes
###############################################################################
predict(cvfit, xtest, ytest = ytest)
#>
#> Call:
#> predict.cv.ptLasso(cvfit = cvfit, xtest = xtest, ytest = ytest)
#>
#>
#>
#> alpha =  0.1
#>
#> Performance (Misclassification error):
```

```
#>
#>             overall   mean group_1 group_2 group_3 group_4 group_5
#> Overall       0.764
#> Pretrain      0.758 0.2008   0.204     0.2     0.2     0.2     0.2
#> Individual    0.800 0.2000   0.200     0.2     0.2     0.2     0.2
#>
#> Support size:
#>
#> Overall    64
#> Pretrain   26 (26 common + 0 individual)
#> Individual 0

################################################################################
# Predict using a separate alpha for each class
################################################################################
predict(cvfit, xtest, ytest = ytest, alphatype = "varying")
#>
#> Call:
#> predict.cv.ptLasso(cvfit = cvfit, xtest = xtest, ytest = ytest,
#>     alphatype = "varying")
#>
#>
#> alpha =  0.1 0.5 0.4 0 0.2
#>
#> Performance (Misclassification error):
#>
#>             overall   mean group_1 group_2 group_3 group_4 group_5
#> Overall       0.764
#> Pretrain      0.770 0.2008   0.204     0.2     0.2     0.2     0.2
#> Individual    0.800 0.2000   0.200     0.2     0.2     0.2     0.2
#>
#> Support size:
#>
#> Overall    64
#> Pretrain   36 (26 common + 10 individual)
#> Individual 0
```

6.2 Time series data

We may have repeated measurements of X and y across time; for example, we may observe patients at two different points in time. We expect that the relationship between X and y will be different at time 1 and time 2, but not completely unrelated. Therefore, pretraining can be useful: we can use the model fitted at time 1 to inform the model for time 2.

`ptLasso` does not natively support this setting, but we can use pretraining nonetheless – below is an example. We assume that X has changed between times 1 and 2. However, if X is constant across time, we can also treat this as a multitask problem – see the section "Multitask learning or coaching" for an example.

To do pretraining, our plan is as follows:

1. fit a model for time 1 and extract its offset and support,
2. use the offset and support (the usual pretraining) to train a model for time 2.

We'll start by simulating data – more details in the comments.

```
set.seed(1234)

n = 600; ntrain = 300;
p = 20

# We assume that X at time 1 (x1) and X at time 2 (x2) are related:
# to get X2, we modify X1.
x1 = matrix(rnorm(n*p), n, p)
x2 = x1 + matrix(0.2 * rnorm(n*p), n, p)

# The relationship between X and y at time 1 and 2 will be similarly related.
# The coefficients at time 2 are a function of those at time 1.
# Importantly, they share the same support.
beta1 = c(rep(2, 10), rep(0, p-10))
beta2 = runif(p, 0.5, 1)*beta1

# Finally, we compute y.
# y2 is a function of y1, x2 and beta2.
y1 = x1 %*% beta1 + rnorm(n)
y2 = 0.5 * y1 + x2 %*% beta2 + rnorm(n)
```

Split into train and test, and define folds to use for cross validation:

```
# Split into train and test:
x1test = x1[-(1:ntrain), ]
x2test = x2[-(1:ntrain), ]
y1test = y1[-(1:ntrain)]
y2test = y2[-(1:ntrain)]

x1 = x1[1:ntrain, ]
x2 = x2[1:ntrain, ]
y1 = y1[1:ntrain]
y2 = y2[1:ntrain]

# Define 10 training folds:
nfolds = 10
foldid = sample(rep(1:10, trunc(nrow(x1)/nfolds)+1))[1:nrow(x1)]
```

The first step is to fit a model for time 1 and extract the cross-fitted offset and support. Note that `cv.glmnet` will store cross-fitted predictions if we use the argument `keep = TRUE`.

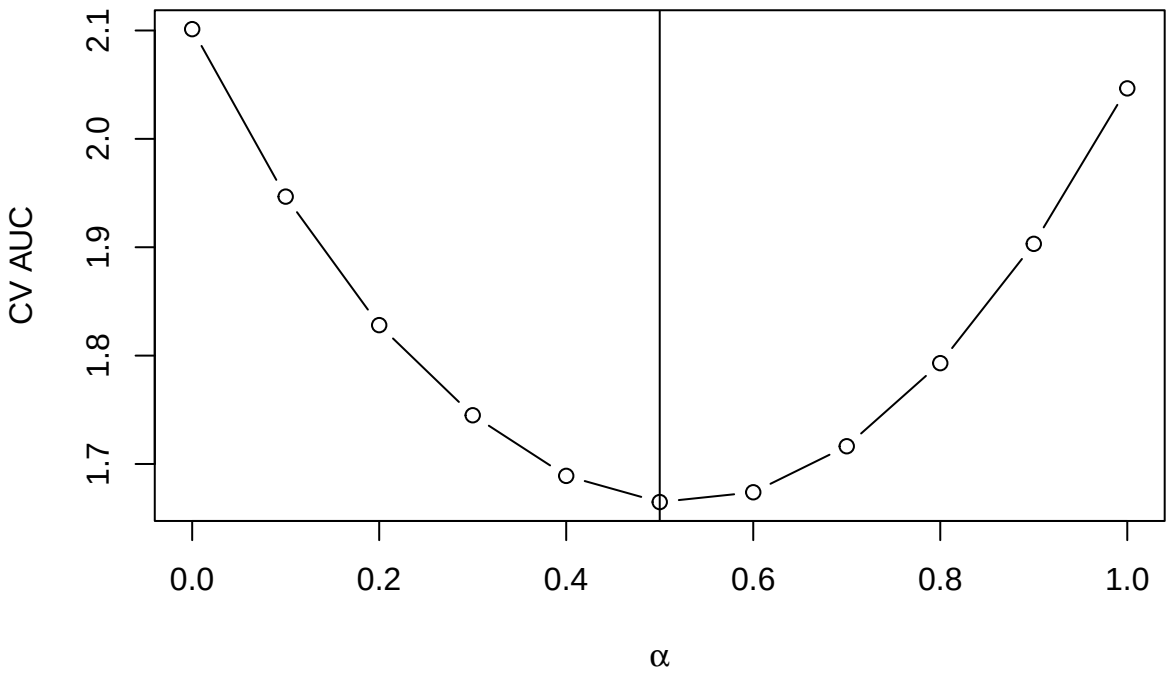
```
y1_fit = cv.glmnet(x1, y1, keep=TRUE, foldid = foldid)

# Identify the support: coefficients which are nonzero:
support = which(coef(y1_fit, s = y1_fit$lambda.1se)[-1] != 0)

# Glmnet computed the cross-fitted predictions:
offset = y1_fit$fit.preval[, y1_fit$lambda == y1_fit$lambda.1se]
```

The last step is to train a model for time 2 using the offset and support from the previous model. As always with pretraining, there is a hyperparameter α that determines the influence of the time 1 model on the time 2 model; we can choose this with cross validation. Here, we train models for a range of values of α (0, 0.1, 0.2, ... 1), and store the cross validated MSE – we will choose α corresponding to the model with the lowest CV MSE.

```
cv.error = NULL
alphalist = seq(0, 1, length.out = 11)

for(alpha in alphalist){
  # Penalty factor:
  pf = rep(1/alpha, p)
  pf[support] = 1

  # Offset:
  offset.alpha = (1 - alpha) * offset

  # Model fitting:
  y2_fit = cv.glmnet(x2, y2,
                     foldid = foldid,
                     offset = offset.alpha,
                     penalty.factor = pf)

  # Use the CV MSE computed by cv.glmnet:
  cv.error = c(cv.error, min(y2_fit$cvm))
}
```

Which α gave us the best performance? Plotting the CV MSE across all αs we compared reveals that the best $\alpha = 0.5$.

```
plot(alphalist, cv.error, type = "b",
     xlab = expression(alpha),
     ylab = "CV AUC")
best.alpha = alphalist[which.min(cv.error)]
abline(v = alphalist[which.min(cv.error)])
```




```
# Train a model using alpha = 0.5
pf = rep(1/best.alpha, p)
pf[support] = 1
```

```
offset.alpha = (1-best.alpha) * offset

y2_fit = cv.glmnet(x2, y2, foldid = foldid,
                   offset = offset.alpha,
                   penalty.factor = pf)
```

Out of curiosity, let's train an entirely separate model for time 2 (though we have done this already – this is the special case of pretraining where $\alpha = 1$). This will give us a baseline performance measure.

```
y2_fit_no_pretrain = cv.glmnet(x2, y2, foldid = foldid)

testoffset = (1 - best.alpha) * predict(y1_fit, x1test, s="lambda.1se")
pretrain_preds = predict(y2_fit, x2test, newoffset = testoffset)
cat("Pretrain PSE:", round(mean((y2test - pretrain_preds)^2), 2), "\n")
#> Pretrain PSE: 1.35

individual_preds = predict(y2_fit_no_pretrain, x2test)
cat("Individual PSE:", round(mean((y2test - individual_preds)^2), 2))
#> Individual PSE: 1.7
```

Pretraining gives us a 20% lower PSE than just using individual models. This is not surprising – we simulated data to favor pretraining. Recall, however, that if the true models at times 1 and 2 are unrelated, cross validation over the pretraining hyperparameter α will encourage us to choose the individual model, and pretraining should not hurt our performance.

6.3 Multi-response data with mixed response types

Muti-response data consists of datasets with covariates X and multiple outcomes $y_1, y_2, y_3, \ldots$. If these outcomes are all continuous, then it may be natural to treat this as a multitask learning problem (see the section "Multitask Learning or Coaching"). If the outcomes have mixed types however – e.g. y_1 is continuous, y_2 binary and y_3 survival – then the problem is slightly more challenging, because there are fewer methods developed for this setting.

Pretraining is a natural fit for this task: we often believe that there is shared information between y_1, y_2 and y_3. If we fit 3 separate models, we never get to take advantage of any shared information; further, because the outcomes have different types, there are very few methods to fit *one* model for all outcomes (an "overall model").

So, we will use pretraining to pass information between models. Our plan is similar to the time series example; we will:

1. fit a model for y_1,
2. extract the offset and support from this model,
3. use the offset and support (the usual pretraining) to train models for y_2 and y_3.

There is one small detail here: we must choose the primary outcome y_1. This is an important choice because it will form the support and offset for the other two outcomes. We recommend making this selection using domain knowledge, but cross-validation (or a validation set) can of course be used.

Here, we walk through an example with simulated data with three outcomes y_1, y_2 and y_3. The 3 outcomes have an overlapping support; the first 10 features are shared. Outcomes 2 and 3 additionally have 5 features unique to them. We'll define y_1 to be continuous, y_2 to be binomial and y_3 to be survival.

```
set.seed(1234)

n = 600; ntrain = 300
p = 50
```

```
x = matrix(rnorm(n*p), n, p)

# y1: continuous response
beta1 = c(rep(.5, 10), rep(0, p-10))
y1 = x %*% beta1 + rnorm(n)

# y2: binomial response
beta2 = runif(p, min = 0.5, max = 1) * beta1  # Shared with group 1
beta2 = beta2 + c(rep(0, 10),
                  runif(5, min = 0, max = 0.5),
                  rep(0, p-15)) # Individual
y2 = rbinom(n, 1, prob = 1/(1 + exp(-x %*% beta2)))

# y3: survival response
beta3 = beta1  # Shared with group 1
beta3 = beta3 + c(rep(0, 10),
                  runif(5, min = -0.1, max = 0.1),
                  rep(0, p-15)) # Individual
y3.true = - log(runif(n)) / exp(x %*% beta3)
y3.cens = runif(n)
y3 = Surv(pmin(y3.true, y3.cens), y3.true <= y3.cens)
```

We split into train and test sets, and define training folds:

```
# Split into train and test
xtest = x[-(1:ntrain), ]
y1test = y1[-(1:ntrain)]
y2test = y2[-(1:ntrain)]
y3test = y3[-(1:ntrain), ]

x = x[1:ntrain, ]
y1 = y1[1:ntrain]
y2 = y2[1:ntrain]
y3 = y3[1:ntrain, ]

# Define training folds
nfolds = 10
foldid = sample(rep(1:10, trunc(nrow(x)/nfolds)+1))[1:nrow(x)]
```

For the first step of pretraining, train a model for the primary outcome (y_1) and record the offset and support – these will be used when training the models for y_2 and y_3.

```
y1_fit = cv.glmnet(x, y1, keep=TRUE, foldid = foldid)

train_offset = y1_fit$fit.preval[, y1_fit$lambda == y1_fit$lambda.1se]
support = which(coef(y1_fit, s = y1_fit$lambda.1se)[-1] != 0)
```

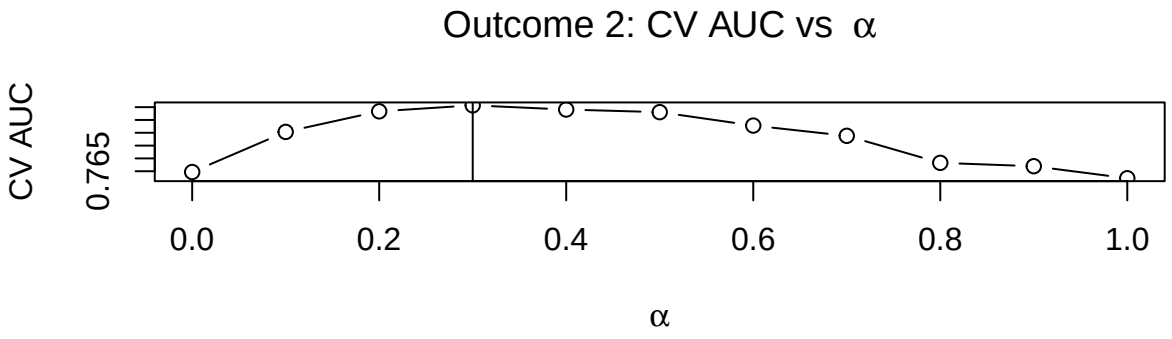
Now we have everything we need to train the models for y_2 and y_3. In the following code, we loop over $\alpha = 0, 0.1, \ldots, 1$; in each step, we (1) train models for y_2 and y_3 and (2) record the CV error from both models. The CV error will be used to determine values of α to use for the final models.

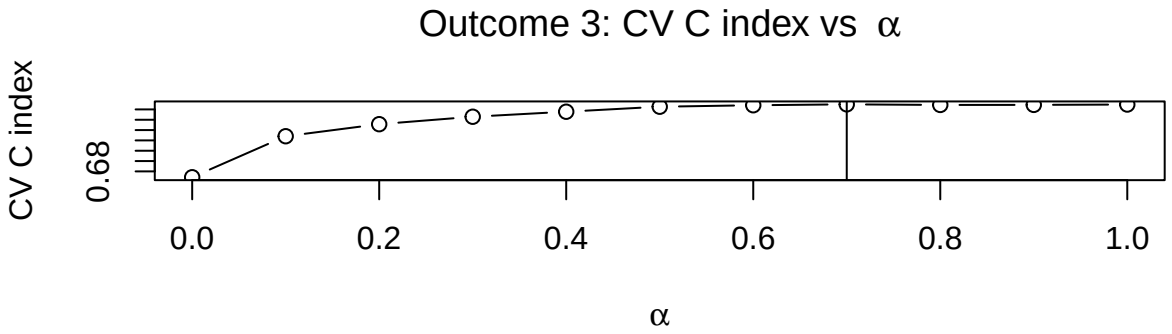
```
cv.error.y2 = cv.error.y3 = NULL
alphalist = seq(0, 1, length.out = 11)

for(alpha in alphalist){
```

```
  pf = rep(1/alpha, p)
  pf[support] = 1

  offset = (1 - alpha) * train_offset

  y2_fit = cv.glmnet(x, y2,
                     foldid = foldid,
                     offset = offset,
                     penalty.factor = pf,
                     family = "binomial",
                     type.measure = "auc")
  cv.error.y2 = c(cv.error.y2, max(y2_fit$cvm))

  y3_fit = cv.glmnet(x, y3,
                     foldid = foldid,
                     offset = offset,
                     penalty.factor = pf,
                     family = "cox",
                     type.measure = "C")
  cv.error.y3 = c(cv.error.y3, max(y3_fit$cvm))
}
```

Plotting our CV performance suggests the value of α we should choose for each outcome:

```
par(mfrow = c(2, 1))
plot(alphalist, cv.error.y2, type = "b",
     main = bquote("Outcome 2: CV AUC vs " ~ alpha),
     xlab = expression(alpha),
     ylab = "CV AUC")
abline(v = alphalist[which.max(cv.error.y2)])

plot(alphalist, cv.error.y3, type = "b",
     main = bquote("Outcome 3: CV C index vs " ~ alpha),
     xlab = expression(alpha),
     ylab = "CV C index")
abline(v = alphalist[which.max(cv.error.y3)])
```





Fit the final models for y_2 and y_3:

```
############################################################
# Model for y2:
############################################################
best.alpha.y2 = alphalist[which.max(cv.error.y2)]
cat("Chosen alpha (y_2):", best.alpha.y2)
#> Chosen alpha (y_2): 0.3

pf = rep(1/best.alpha.y2, p); pf[support] = 1

y2_fit = cv.glmnet(x, y2,
                   foldid = foldid,
                   offset = (1-best.alpha.y2) * train_offset,
                   penalty.factor = pf,
                   family = "binomial",
                   type.measure = "auc")

############################################################
# Repeat for y3:
############################################################
best.alpha.y3 = alphalist[which.max(cv.error.y3)]
cat("Chosen alpha (y_3):", best.alpha.y3)
#> Chosen alpha (y_3): 0.7

pf = rep(1/best.alpha.y3, p); pf[support] = 1

y3_fit = cv.glmnet(x, y3,
                   foldid = foldid,
                   offset = (1-best.alpha.y3) * train_offset,
```

```
                    penalty.factor = pf,
                    family = "cox",
                    type.measure = "C")
```

We will also train models for y_2 and y_3 *without* pretraining; this is a natural benchmark.

```
y2_fit_no_pretrain = cv.glmnet(x, y2, foldid = foldid,
                               family = "binomial", type.measure = "auc")

y3_fit_no_pretrain = cv.glmnet(x, y3,
                               foldid = foldid,
                               family = "cox", type.measure = "C")
```

All of our models have been trained. Let's compare performance with and without pretraining; we'll start with the model for y_2.

```
testoffset = predict(y1_fit, xtest, s = "lambda.1se")

cat("Model 2 AUC with pretraining:",
    round(assess.glmnet(y2_fit, xtest, newy = y2test,
                        newoffset = (1 - best.alpha.y2) * testoffset)$auc, 2),
    fill=TRUE)
#> Model 2 AUC with pretraining: 0.76

cat("Model 2 AUC without pretraining:",
    round(assess.glmnet(y2_fit_no_pretrain, xtest, newy = y2test)$auc, 2)
    )
#> Model 2 AUC without pretraining: 0.66
```

And now, the models for y_3:

```
cat("Model 3 C-index with pretraining:",
    round(assess.glmnet(y3_fit, xtest, newy = y3test,
                        newoffset = (1 - best.alpha.y3) * testoffset)$C, 2))
#> Model 3 C-index with pretraining: 0.8

cat("Model 3 C-index without pretraining:",
    round(assess.glmnet(y3_fit_no_pretrain, xtest, newy = y3test)$C, 2)
    )
#> Model 3 C-index without pretraining: 0.78
```

For both y_2 and y_3, we saw a performance improvement using pretraining. We didn't technically need to train the individual (non-pretrained) models for y_2 and y_3: during our CV loop to choose α, we saw the cross validation performance for the individual models (the special case when $\alpha = 1$), and CV recommended a smaller value of α for both outcomes.

Note that, in this example, we trained a model using y_1, and then used this model to form the offset and support for the models for y_2 and y_3 in parallel. But using pretraining for multi-response data is *flexible*. Pretraining is simply a method to pass information from one model to another, and we are free to choose how information flows. For example, we chose to pass information from model 1 (y_1) to model 2 (y_2) and to model 3 (y_3). But, we could have instead *chained* our models to pass information from model 1 to model 2, and then from model 2 to model 3 in the following way:

1. fit a model for y_1,
2. extract the offset and support from this model,
3. use the offset and support (the usual pretraining) to train a model for y_2,
4. extract the offset and support from this second model, and

5. use them to train a model for y_3.

In this framework, the model for y_3 depends implicitly on both the models for y_1 *and* y_2, as the offset and support for the model for y_2 were informed by the model for y_1. Choosing how information should be passed between outcomes is context specific and we recommend relying on domain knowledge for selecting an approach (though many options may be tried and compared with cross-validation or a validation set).

6.4 Multi-task learning or coaching

Multitask learning consists of data X with two or more responses $y_1, \ldots, y_j$. We usually assume that there is shared signal across the responses, and that performance can be improved by jointly fitting models for the responses.

Pretraining is a natural choice for multitask learning – it is a method to pass information between models. The overview for our approach is to:

1. fit a multi-response Gaussian model,
2. extract the support (shared across responses) and offsets (one for each response), and
3. fit a model for each response, using the shared support and appropriate offset.

We will illustrate this with simulated data with two Gaussian responses; the two responses share the first 5 features, and they each have 5 features of their own. The two responses are quite related, with Pearson correlation around 0.5.

```
set.seed(1234)

n = 1000; ntrain = 500;
p = 500
sigma = 2

x = matrix(rnorm(n*p), n, p)
beta1 = c(rep(1, 5), rep(0.5, 5), rep(0, p - 10))
beta2 = c(rep(1, 5), rep(0, 5), rep(0.5, 5), rep(0, p - 15))

mu = cbind(x %*% beta1, x %*% beta2)
y  = cbind(mu[, 1] + sigma * rnorm(n),
           mu[, 2] + sigma * rnorm(n))
cat("SNR for the two tasks:", round(diag(var(mu)/var(y-mu)), 2))
#> SNR for the two tasks: 1.6 1.44

xtest = x[-(1:ntrain), ]
ytest = y[-(1:ntrain), ]

x = x[1:ntrain, ]
y = y[1:ntrain, ]

# Define training folds
nfolds = 5
foldid = sample(rep(1:nfolds, trunc(nrow(x)/nfolds)+1))[1:nrow(x)]

cat("Correlation between two tasks:", cor(y[, 1], y[, 2]))
#> Correlation between two tasks: 0.5218575
```

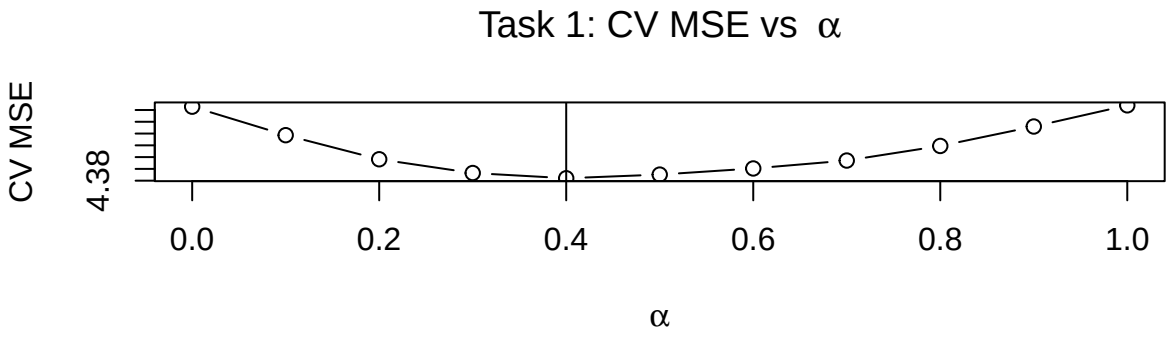
The first step of pretraining is to fit a multi-response Gaussian model and extract the offset and support.

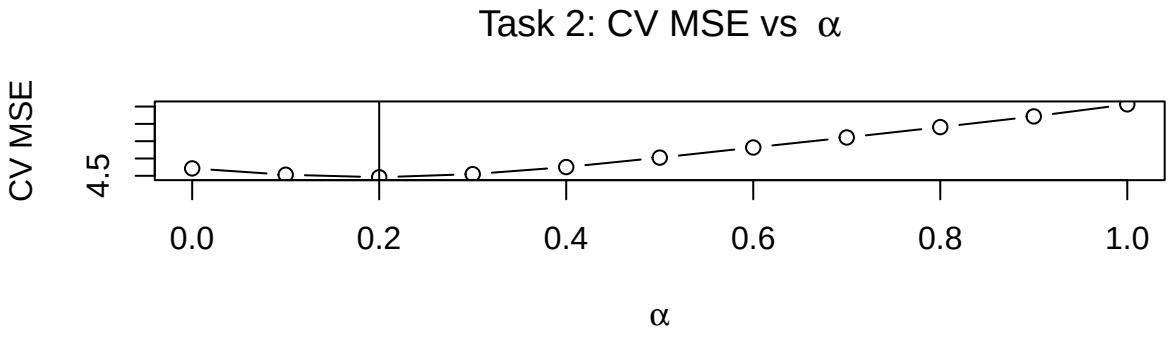
```
mtask.fit = cv.glmnet(x, y, family = "mgaussian",
                      keep = TRUE,
```

```
                      foldid = foldid,
                      type.measure = "mse")

offset = mtask.fit$fit.preval[, , mtask.fit$lambda == mtask.fit$lambda.1se]

coefs = coef(mtask.fit, s = "lambda.1se")
coefs = cbind(coefs$y1, coefs$y2)
support = which((rowSums(coefs) != 0)[-1])
```

And now, we'll fit a separate model for each response. We will loop over values of α $(0, 0.1, \ldots, 1)$; for each α, we fit a model for each response using the offset and support defined above and modified by α. We also record the minimum CV mean squared error for each model – this is how we will perform model selection.

```
cv.error = c(NULL, NULL)
alphalist = seq(0, 1, length.out = 11)

for(alpha in alphalist){
  pf = rep(1/alpha, p)
  pf[support] = 1

  y1_fit = cv.glmnet(x, y[, 1],
                     foldid = foldid,
                     offset = (1 - alpha) * offset[, 1],
                     penalty.factor = pf,
                     family = "gaussian",
                     type.measure = "mse")

  y2_fit = cv.glmnet(x, y[, 2],
                     foldid = foldid,
                     offset = (1 - alpha) * offset[, 2],
                     penalty.factor = pf,
                     family = "gaussian",
                     type.measure = "mse")

  cv.error = rbind(cv.error, c(min(y1_fit$cvm), min(y2_fit$cvm)))
}

par(mfrow = c(2, 1))
plot(alphalist, cv.error[, 1], type = "b",
     xlab = expression(alpha), ylab = "CV MSE",
     main = bquote("Task 1: CV MSE vs " ~ alpha))
abline(v = alphalist[which.min(cv.error[, 1])])

plot(alphalist, cv.error[, 2], type = "b",
     xlab = expression(alpha), ylab = "CV MSE",
     main = bquote("Task 2: CV MSE vs " ~ alpha))
abline(v = alphalist[which.min(cv.error[, 2])])
```





The optimal values of α for the two responses are pretty close, and we could choose to use one α for both responses (say, the α that minimizes the average CV for both class). Here, we will choose to use two separate values of α. We train our final models:

```
best.alpha.1 = alphalist[which.min(cv.error[, 1])]
best.alpha.2 = alphalist[which.min(cv.error[, 2])]

pf = rep(1/best.alpha.1, p)
pf[support] = 1
y1_fit = cv.glmnet(x, y[, 1], foldid = foldid,
                   offset = (1 - best.alpha.1) * offset[, 1],
                   penalty.factor = pf,
                   family = "gaussian",
                   type.measure = "mse")

pf = rep(1/best.alpha.2, p)
pf[support] = 1
y2_fit = cv.glmnet(x, y[, 2], foldid = foldid,
                    offset = (1 - best.alpha.2) * offset[, 2],
                    penalty.factor = pf,
                    family = "gaussian",
                    type.measure = "mse")
```

There are two natural baselines: one is the performance of the multi-response model used in the first step of pretraining, and the other is a separate model for each response:

```
y1_fit_no_pretrain = cv.glmnet(x, y[, 1], foldid = foldid,
                               family = "gaussian", type.measure = "mse")

y2_fit_no_pretrain = cv.glmnet(x, y[, 2], foldid = foldid,
                               family = "gaussian", type.measure = "mse")
```

Compare performance for task 1:

```
test_offset = predict(mtask.fit, xtest, s = "lambda.1se")[, , 1]

test_mtask_pred = predict(mtask.fit, xtest, s = "lambda.min")[, , 1]

cat("Response 1 MSE overall model:",
    round(assess.glmnet(test_mtask_pred[, 1], newy = ytest[, 1])$mse, 2))
#> Response 1 MSE overall model: 4.25

cat("Response 1 MSE with pretraining:",
    round(assess.glmnet(y1_fit, xtest, newy = ytest[, 1],
                        newoffset = (1 - best.alpha.1) * test_offset[, 1])$mse,
          2))
#> Response 1 MSE with pretraining: 4.26

cat("Response 1 MSE individual model:",
    round(assess.glmnet(y1_fit_no_pretrain, xtest, newy = ytest[, 1])$mse, 2))
#> Response 1 MSE individual model: 4.48
```

And performance for task 2:

```
cat("Response 2 MSE overall model:",
    round(assess.glmnet(test_mtask_pred[, 2], newy = ytest[, 2])$mse, 2))
#> Response 2 MSE overall model: 5.21

cat("Model 2 MSE with pretraining:",
    round(assess.glmnet(y2_fit, xtest, newy = ytest[, 2],
                        newoffset = (1 - best.alpha.2) * test_offset[, 2])$mse,
          2))
#> Model 2 MSE with pretraining: 4.98

cat("Model 2 MSE individual model:",
    round(assess.glmnet(y2_fit_no_pretrain, xtest, newy = ytest[, 2])$mse, 2))
#> Model 2 MSE individual model: 5.8
```

We find that pretraining improves performance for response 2, and has performance close to that of the overall model for response 1.

7 Conditional average treatment effect estimation

7.1 Background: CATE estimation and pretraining

In causal inference, we are often interested in predicting the treatment effect for individual observations; this is called the conditional average treatment effect (CATE). For example, before prescribing a drug to a patient, we want to know whether the drug is likely to work well *for that patient* - not just whether it works well on average. One tool to model the CATE is the R-learner (Nie and Wager (2021)), which minimizes the R loss:

$$\hat{L}_n\{\tau(\cdot)\} = \arg\min_{\tau} \frac{1}{n} \sum \Big[(y_i - m^*(x_i)) - (W_i - e^*(x_i))\tau(x_i) \Big]^2.$$

Here, x_i and y_i are the covariates and outcome for observation i, $e^*(x_i)$ is the treatment propensity and W_i the treatment assignment, and $m^*(x_i)$ is the conditional mean outcome ($E[y_i \mid x = x_i]$). Then, $\hat{\tau}$ is the estimate of the heterogeneous treatment effect function.

This is fitted in stages: first, the R-learner fits m^* and e^* to get $\hat{m}^*$ and $\hat{e}^*$; then plugs in $\hat{m}^*(x_i)$ and $\hat{e}^*(x_i)$

to fit τ. A minor detail is that cross-fitting (or prevalidation) is used in the first stage so that the plugin value for e.g. $\hat{m}^*(x_i)$ comes from a model trained without using x_i.

When τ is a linear function, then the second stage of fitting is straightforward. The values $\hat{m}^*(x_i)$ and $\hat{e}^*(x_i)$ are known, and we can use linear regression to model $y_i - \hat{m}^*(x_i)$ as a function of the weighted feature vector $(W_i - \hat{e}^*(x_i))x_i$. This is what we will do in the following example.

How can pretraining be useful here? Well, we are separately fitting models for m^* (the conditional mean) and τ (the heterogeneous treatment effect), and these two functions are likely to share support: it is sensible to assume that the features that modulate the mean treatment effect also modulate the heterogeneous treatment effect. We can use pretraining by (1) training a model for m^* and (2) using the support from this model to guide the fitting of τ. Note that the offset is not used in this case; m^* and τ are designed to predict different outcomes.

7.2 A simulated example

Here is an example. We will simplify the problem by assuming treatment has been randomized – the true $e^*(x_i) = 0.5$ for all i.

```
set.seed(1234)

n = 600; ntrain = 300
p = 20

x = matrix(rnorm(n*p), n, p)

# Treatment assignment
w = rbinom(n, 1, 0.5)

# m^*
m.coefs = c(rep(2,10), rep(0, p-10))
m = x %*% m.coefs

# tau
tau.coefs = runif(p, 0.5, 1)*m.coefs
tau = 1.5*m + x%*%tau.coefs

mu = m + w * tau
y  = mu + 10 * rnorm(n)
cat("Signal to noise ratio:", var(mu)/var(y-mu))
#> Signal to noise ratio: 2.301315

# Split into train/test
xtest = x[-(1:ntrain), ]
tautest = tau[-(1:ntrain)]
wtest = w[-(1:ntrain)]

x = x[1:ntrain, ]
y = y[1:ntrain]
w = w[1:ntrain]

# Define training folds
nfolds = 10
foldid = sample(rep(1:10, trunc(nrow(x)/nfolds)+1))[1:nrow(x)]
```

We begin model fitting, starting with our estimate of e^* (the probability of receiving the treatment). To fit τ,

we will also need to record the cross-fitted $\hat{e}^*(x)$.

```
e_fit = cv.glmnet(x, w, foldid = foldid,
                  family="binomial", type.measure="deviance",
                  keep = TRUE)

e_hat = e_fit$fit.preval[, e_fit$lambda == e_fit$lambda.1se]
e_hat = 1/(1 + exp(-e_hat))
```

Now, stage 1 of pretraining: fit a model for m^* and record the support. As before, we also record the cross-fitted $\hat{m}^*(x)$.

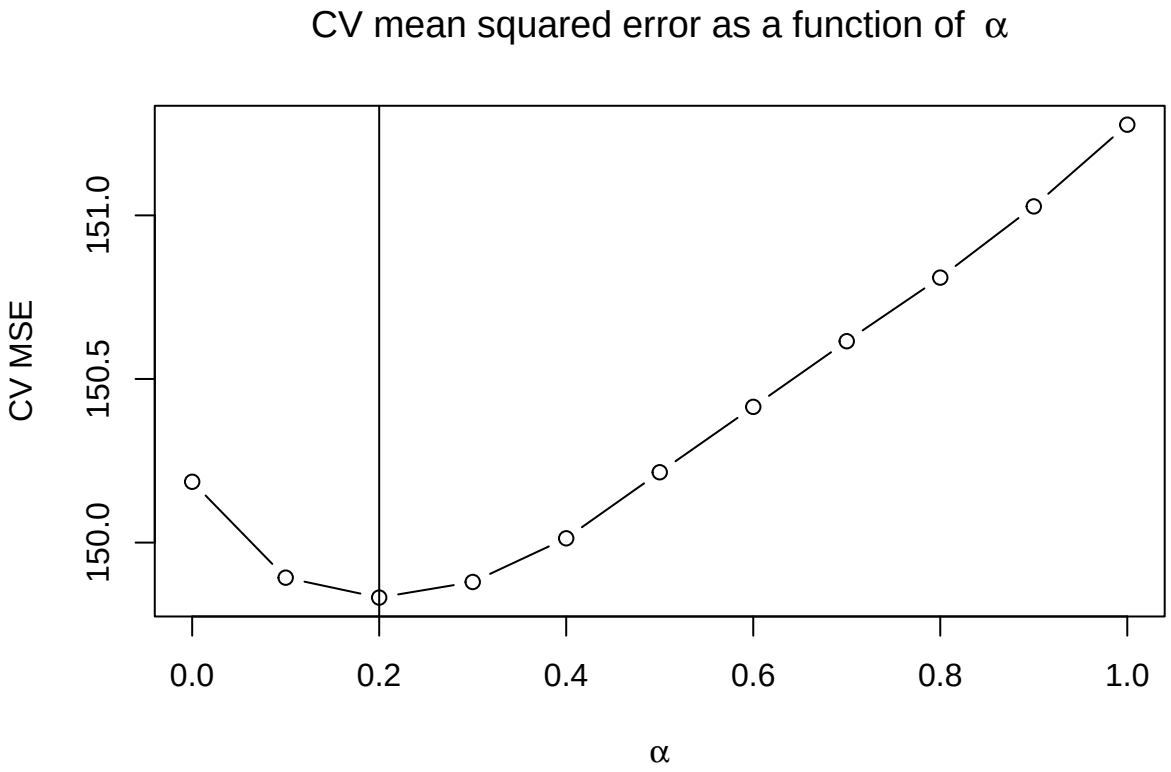
```
m_fit = cv.glmnet(x, y, foldid = foldid, keep = TRUE)

m_hat = m_fit$fit.preval[, m_fit$lambda == m_fit$lambda.1se]

bhat = coef(m_fit, s = m_fit$lambda.1se)
support = which(bhat[-1] != 0)
```

To fit τ, we will regress $\tilde{y} = y_i - \hat{m}^*(x_i)$ on $\tilde{x} = (w_i - \hat{e}^*(x_i))x_i$; we'll define them here:

```
y_tilde = y - m_hat
x_tilde = cbind(as.numeric(w - e_hat) * cbind(1, x))
```

And now, pretraining for τ. Loop over $\alpha = 0, 0.1, \ldots, 1$; for each α, fit a model for τ using the penalty factor defined by the support of $\hat{m}$ and α. We'll keep track of our CV MSE at each step so that we can choose the α that minimizes the MSE.

```
cv.error = NULL
alphalist = seq(0, 1, length.out = 11)

for(alpha in alphalist){
  pf = rep(1/alpha, p)
  pf[support] = 1
  pf = c(0, pf) # Don't penalize the intercept

  tau_fit = cv.glmnet(x_tilde, y_tilde,
                      foldid = foldid,
                      penalty.factor = pf,
                      intercept = FALSE, # already include in x_tilde
                      standardize = FALSE)
  cv.error = c(cv.error, min(tau_fit$cvm))
}


plot(alphalist, cv.error, type = "b",
     xlab = expression(alpha),
     ylab = "CV MSE",
     main = bquote("CV mean squared error as a function of " ~ alpha))
abline(v = alphalist[which.min(cv.error)])
```



In the plot above, the value at $\alpha = 1$ corresponds to the usual R learner, which makes no assumption about a shared support between τ and m^*. Based on the plot, we choose $\alpha = 0.2$ as our best performing model:

```
best.alpha = alphalist[which.min(cv.error)]
cat("Chosen alpha:", best.alpha)
#> Chosen alpha: 0.2

pf = rep(1/best.alpha, p)
pf[support] = 1
pf = c(0, pf)
tau_fit = cv.glmnet(x_tilde, y_tilde, foldid = foldid,
                    penalty.factor = pf,
                    intercept = FALSE,
                    standardize = FALSE)
```

To concretely compare the pretrained R-learner with the usual R-learner, we'll train the usual R-learner here:

```
tau_rlearner = cv.glmnet(x_tilde, y_tilde, foldid = foldid,
                         penalty.factor = c(0, rep(1, ncol(x))),
                         intercept = FALSE,
                         standardize = FALSE)
```

As anticipated, pretraining improves the prediction squared error relative to the R learner – this is how we designed our simulation:

```
rlearner_preds   = predict(tau_rlearner, cbind(1, xtest), s = "lambda.min")
cat("R-learner PSE: ",
    round(mean((rlearner_preds - tautest)^2), 2))
#> R-learner PSE:  45.85

pretrained_preds = predict(tau_fit, cbind(1, xtest), s = "lambda.min")
```

```
cat("Pretrained R-learner PSE: ",
    round(mean((pretrained_preds - tautest)^2), 2))
#> Pretrained R-learner PSE:  37.63
```

7.3 What if the pretraining assumption is wrong?

Here, we repeat everything from above, only now there is no overlap in the support of m^* and τ.

```
#########################################################
# Simulate data
#########################################################
x = matrix(rnorm(n*p), n, p)

# Treatment assignment
w = rbinom(n, 1, 0.5)

# m^*
m.coefs = c(rep(2,10), rep(0, p-10))
m = x %*% m.coefs

# tau
# Note these coefficients have no overlap with m.coefs!
tau.coefs = c(rep(0, 10), rep(2, 10), rep(0, p-20))
tau = x%*%tau.coefs

mu = m + w * tau
y  = mu + 10 * rnorm(n)
cat("Signal to noise ratio:", var(mu)/var(y-mu))
#> Signal to noise ratio: 0.6938152

# Split into train/test
xtest = x[-(1:ntrain), ]
tautest = tau[-(1:ntrain)]
wtest = w[-(1:ntrain)]

x = x[1:ntrain, ]
y = y[1:ntrain]
w = w[1:ntrain]

#########################################################
# Model fitting: e^*
#########################################################
e_fit = cv.glmnet(x, w, foldid = foldid,
                  family="binomial", type.measure="deviance",
                  keep = TRUE)
e_hat = e_fit$fit.preval[, e_fit$lambda == e_fit$lambda.1se]
e_hat = 1/(1 + exp(-e_hat))

#########################################################
# Model fitting: m^*
#########################################################
m_fit = cv.glmnet(x, y, foldid = foldid, keep = TRUE)

m_hat = m_fit$fit.preval[, m_fit$lambda == m_fit$lambda.1se]
```

```r
bhat = coef(m_fit, s = m_fit$lambda.1se)
support = which(bhat[-1] != 0)

#########################################################
# Pretraining: tau
#########################################################
y_tilde = y - m_hat
x_tilde = cbind(as.numeric(w - e_hat) * cbind(1, x))

cv.error = NULL
alphalist = seq(0, 1, length.out = 11)

for(alpha in alphalist){
  pf = rep(1/alpha, p)
  pf[support] = 1
  pf = c(0, pf) # Don't penalize the intercept

  tau_fit = cv.glmnet(x_tilde, y_tilde,
                      foldid = foldid,
                      penalty.factor = pf,
                      intercept = FALSE, # already include in x_tilde
                      standardize = FALSE)
  cv.error = c(cv.error, min(tau_fit$cvm))
}

# Our final model for tau:
best.alpha = alphalist[which.min(cv.error)]
cat("Chosen alpha:", best.alpha)
#> Chosen alpha: 1

pf = rep(1/best.alpha, p)
pf[support] = 1
pf = c(0, pf)
tau_fit = cv.glmnet(x_tilde, y_tilde, foldid = foldid,
                    penalty.factor = pf,
                    intercept = FALSE,
                    standardize = FALSE)

#########################################################
# Fit the usual R-learner:
#########################################################
tau_rlearner = cv.glmnet(x_tilde, y_tilde, foldid = foldid,
                         penalty.factor = c(0, rep(1, ncol(x))),
                         intercept = FALSE,
                         standardize = FALSE)

#########################################################
# Measure performance:
#########################################################
rlearner_preds = predict(tau_rlearner, cbind(1, xtest), s = "lambda.min")
cat("R-learner prediction squared error: ",
    round(mean((rlearner_preds - tautest)^2), 2))
#> R-learner prediction squared error:  31.11
```

```
pretrained_preds = predict(tau_fit, cbind(1, xtest), s = "lambda.min")
cat("Pretrained R-learner prediction squared error: ",
    round(mean((pretrained_preds - tautest)^2), 2))
#> Pretrained R-learner prediction squared error:  31.11
```

Pretraining has not hurt our performance, even though the support of m^* and τ are not shared. Why? Recall that we defined $y = m^*(x) + W * \tau(x) + \epsilon$, so the relationship between y and x is a function of the supports of both m^* and τ. In the first stage of pretraining, we fitted m^* using `y ~ x` – so the support of m^* *should* include the support of τ. As a result, using pretraining with the R-learner should not harm predictive performance.

8 Using non-linear bases

Suppose we have a dataset with features X and response y, where the relationship between X and y is a nonlinear function of the columns of X. Can we still use the lasso? Yes! We can *pretrain* our linear model using `xgboost` to obtain basis functions (features). Let's walk through an example.

8.1 Example 1: xgboost pretraining

```
require(xgboost)
#> Loading required package: xgboost
```

We start by simulating data ($n = 1800$, $p = 1000$) with a continuous response. Our coefficients β are sparse; the first 200 entries will be drawn from a standard univariate normal, and the remainder are 0. We define y as $y = 1(X > 0)\beta + \epsilon$, where ϵ is noise; we hope that `xgboost` will learn the splits corresponding to $X > 0$.

```
set.seed(1234)

n = 1800; p = 1000; noise = 5;

x     = matrix(rnorm(n * p), nrow=n, ncol=p)
xtest = matrix(rnorm(n * p), nrow=n, ncol=p)

x.model     = 1*(x > 0)
xtest.model = 1*(xtest > 0)

beta = c(rnorm(200), rep(0, p-200))

y     = x.model %*% beta + noise * rnorm(n)
ytest = xtest.model %*% beta + noise * rnorm(n)

train.folds = sample(rep(1:10, n/10))
```

Now, we run `xgboost` to get our basis functions:

```
xgbfit      = xgboost(data=x, label=y, nrounds=200, max_depth=1, verbose=0)

x.boost     = predict(xgbfit, x, predleaf = TRUE) - 1
xtest.boost = predict(xgbfit, xtest, predleaf = TRUE) - 1
```

And we are ready for model fitting with `cv.glmnet`. Our two baselines are (1) a linear model that does not pretrain with `xgboost`, and (2) `xgboost`. We find that `glmnet` together with `xgboost` outperforms `glmnet` alone and `xgboost` alone.

Table 3: Coefficients for simulating data for use with xgboost pretraining

	1-50	51-100	101-150	151-200	201-500
group 1	2	1	0	0	0
group 2	2	0	1	0	0
group 3	2	0	0	1	0

```
cvfit = cv.glmnet(x.boost, y, type.measure = "mse", foldid = train.folds)
cvfit.noboost = cv.glmnet(x, y, type.measure = "mse", foldid = train.folds)

cat("Lasso with xgboost pretraining PSE: ",
    assess.glmnet(cvfit, newx = xtest.boost, newy = ytest)$mse)
#> Lasso with xgboost pretraining PSE:  46.23225

cat("Lasso without xgboost pretraining PSE: ",
    assess.glmnet(cvfit.noboost, newx = xtest, newy = ytest)$mse)
#> Lasso without xgboost pretraining PSE:  60.68818

cat("xgboost alone PSE: ",
    assess.glmnet(predict(xgbfit, xtest), newy = ytest)$mse)
#> xgboost alone PSE:  49.47738
```

8.2 Example 2: xgboost pretraining with input groups

Now, let's repeat the above supposing our data have input groups. The only difference here is that we will use `cv.ptLasso` for our model instead of `cv.glmnet`, and we will use the group indicators as a feature when fitting `xgboost`.

We start by simulating data with 3 groups (600 observations in each group) and a continuous response. As before, we will simulate y as $y = 1(X > 0)\beta + \epsilon$, only now we have a different β for each group. The coefficients for the groups are in Table 3.

```
set.seed(1234)

n = 1800; p = 500; k = 3;
noise = 5;

groups = groupstest = sort(rep(1:k, n/k))

x     = matrix(rnorm(n * p), nrow=n, ncol=p)
xtest = matrix(rnorm(n * p), nrow=n, ncol=p)

x.model     = 1*(x > 0)
xtest.model = 1*(xtest > 0)

common.beta = c(rep(2, 50), rep(0, p-50))
beta.1 = c(rep(0, 50),  rep(1, 50), rep(0, p-100))
beta.2 = c(rep(0, 100), rep(1, 50), rep(0, p-150))
beta.3 = c(rep(0, 150), rep(1, 50), rep(0, p-200))

y = x.model %*% common.beta + noise * rnorm(n)
y[groups == 1] = y[groups == 1] + x.model[groups == 1, ] %*% beta.1
```

```
y[groups == 2] = y[groups == 2] + x.model[groups == 2, ] %*% beta.2
y[groups == 3] = y[groups == 3] + x.model[groups == 3, ] %*% beta.3

ytest = xtest.model %*% common.beta + noise * rnorm(n)
ytest[groups == 1] = ytest[groups == 1] + xtest.model[groups == 1, ] %*% beta.1
ytest[groups == 2] = ytest[groups == 2] + xtest.model[groups == 2, ] %*% beta.2
ytest[groups == 3] = ytest[groups == 3] + xtest.model[groups == 3, ] %*% beta.3
```

Here are the dummy variables for our group indicators; we will use them to fit and predict with `xgboost`.

```
group.ids     = model.matrix(~as.factor(groups) - 1)
grouptest.ids = model.matrix(~as.factor(groupstest) - 1)
colnames(grouptest.ids) = colnames(group.ids)
```

Now, let's train `xgboost` and `predict` to get our new features. Note that we now use `max_depth = 2`: this is intended to allow interactions between the group indicators and the other features.

```
xgbfit      = xgboost(data=cbind(x, group.ids), label=y,
                      nrounds=200, max_depth=2, verbose=0)

x.boost     = predict(xgbfit, cbind(x, group.ids), predleaf = TRUE) - 1
xtest.boost = predict(xgbfit, cbind(xtest, grouptest.ids), predleaf = TRUE) - 1
```

Finally, we are ready to fit two models trained with `cv.ptLasso`: one uses the xgboost features and the other does not. As before, we find that pretraining with xgboost improves performance relative to (1) model fitting in the original feature space and (2) xgboost alone.

```
cvfit = cv.ptLasso(x.boost, y, groups=groups, type.measure = "mse")
preds = predict(cvfit, xtest.boost, groups=groupstest, alphatype = "varying")
preds = preds$yhatpre

cvfit.noboost = cv.ptLasso(x, y, groups=groups, type.measure = "mse")
preds.noboost = predict(cvfit.noboost, xtest, groups=groupstest,
                        alphatype = "varying")
preds.noboost = preds.noboost$yhatpre

cat("ptLasso with xgboost pretraining PSE: ",
    assess.glmnet(preds, newy = ytest)$mse)
#> ptLasso with xgboost pretraining PSE:  55.5542

cat("ptLasso without xgboost pretraining PSE: ",
    assess.glmnet(preds.noboost, newy = ytest)$mse)
#> ptLasso without xgboost pretraining PSE:  63.32061

cat("xgboost alone PSE: ",
    assess.glmnet(predict(xgbfit, xtest), newy = ytest)$mse)
#> xgboost alone PSE:  59.63781
```

9 Unsupervised pretraining

Suppose we have a dataset with features X and response y. Suppose we also have a large set of *unlabeled* data X^*. Here, we show how to *pretrain* a model using X^*. The steps are:

1. Do sparse PCA using X^*. Identify the nonzero features in the first principal component (PC).
2. Use `glmnet` (or `cv.glmnet`) to train model using X and y. Define the penalty factor using the support

identified by sparse PCA. Unlike the usual pretraining, there is no offset defined by sparse PCA.

In step 1, we may choose to use the nonzero features from the first k PCs instead of just the first PC; in the examples that follow, we use only the first PC for simplicity.

To demonstrate unsupervised pretraining, we'll use simulated data. The covariates X and X^* are drawn from a multivariate normal distribution where the first 10 features describe most of the variance, and y is defined as $X\beta + \epsilon$, where only the first 10 coefficients in β are nonzero and ϵ is noise. In this example, we have 10 times as much unlabeled data as labeled data; this generally happens when labels are difficult to obtain.

```
require(MASS) # for mvrnorm
#> Loading required package: MASS

set.seed(1234)

n = 100; p = 150;

mu = rep(0, p)
sigma <- matrix(runif(p^2)*2-1, ncol=p)
sigma[, 11:p] = 1e-2 # The first 10 features are the most important
sigma <- t(sigma) %*% sigma
diag(sigma)[11:p] = 1

x     = mvrnorm(n = n, mu = mu, Sigma = sigma)
xtest = mvrnorm(n = n, mu = mu, Sigma = sigma)
xstar = mvrnorm(n = 10 * n, mu = mu, Sigma = sigma) # unlabeled

noise = 3
beta = c(rep(1, 10), rep(0, p - 10))
y     = x %*% beta     + noise * rnorm(n)
ytest = xtest %*% beta + noise * rnorm(n)

train.folds = sample(rep(1:10, 10))
```

Now, we do sparse PCA using X^* and we identify the features with nonzero loadings in the first PC. The argument $k = 1$ means that we only obtain the first PC.

```
require(sparsepca)
#> Loading required package: sparsepca

pcs = spca(xstar, k = 1, verbose=FALSE, alpha=1e-2, beta=1e-2)
nonzero.loadings = which(pcs$loadings != 0)
```

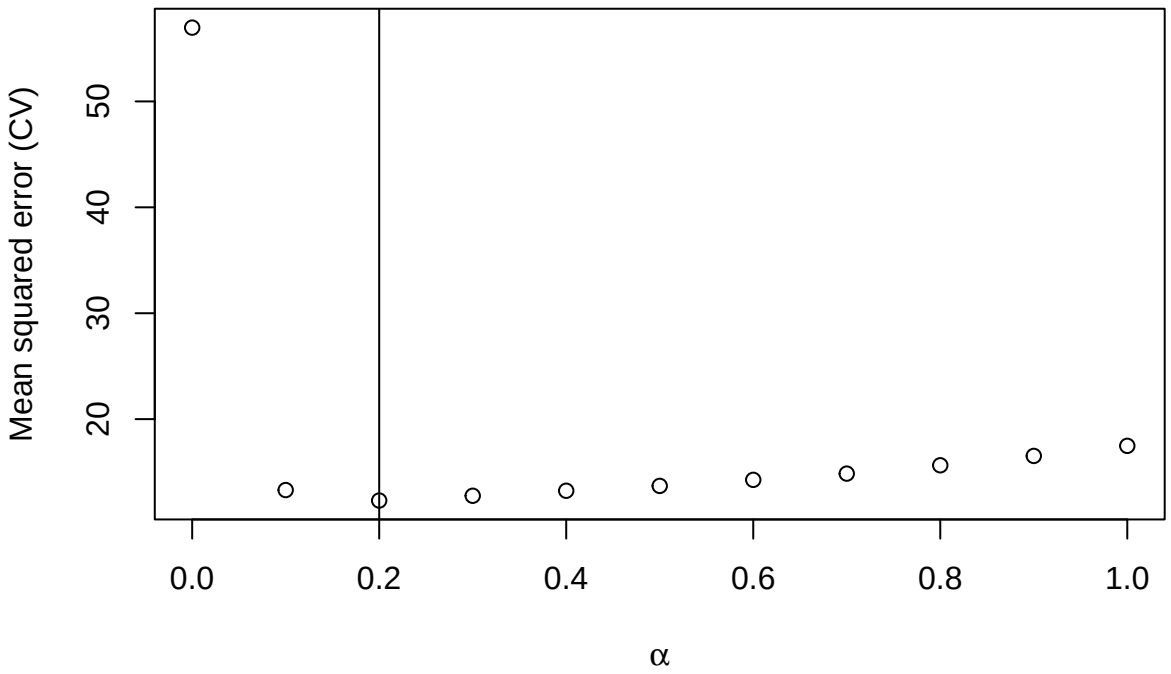
We set ourselves up for success: because of how we simulated our data, we know that the first 10 features are those that explain the variance in X. These are also the features that define the relationship between X and y. Let's check that sparse PCA has found the right features:

```
nonzero.loadings
#> [1]  1  2  3  4  5  6  7  8 10
```

Now, we are ready to model! We don't need to call `ptLasso` here. All we need to do is call `cv.glmnet` across a grid of values of α with a different `penalty.factor` for each call. Note that `offset` is not used – sparse PCA identifies *which features* may important, but it doesn't suggest a value for the fitted coefficients.

To do model selection, we want to know which value of α gave us the best CV error. Fortunately, `cv.glmnet` will record the CV MSE for each model in a vector called `cvm`; we just need to keep track of the minimum error from each model.

```
alphalist = seq(0, 1, length.out = 11)

cvm = NULL
for(alpha in alphalist){
  # Define the penalty factor:
  pf = rep(1/alpha, p)
  pf[nonzero.loadings] = 1

  # Train a model:
  model = cv.glmnet(x, y, family = "gaussian", type.measure = "mse",
                              penalty.factor = pf,
                              foldid = train.folds)

  # Record the minmum CV MSE for this model:
  cvm = c(cvm, min(model$cvm))
}

best.alpha = alphalist[which.min(cvm)]

# Plot performance as a function of alpha
# with a vertical line to show us the minimum mse:
plot(alphalist, cvm,
     xlab = expression(alpha),
     ylab = "Mean squared error (CV)"
)
abline(v = best.alpha)
```



So, using CV performance as a metric, we choose $\alpha = 0.2$. Now, we train our final model and predict and measure performance with our held-out data. We find that pretraining gives us a boost in performance.

```
pf = rep(1/best.alpha, p)
pf[nonzero.loadings] = 1
```

```
selected.model =  cv.glmnet(x, y, family = "gaussian", type.measure = "mse",
                            penalty.factor = pf,
                            foldid = train.folds)

# Prediction squared error with pretraining:
assess.glmnet(selected.model, xtest, newy = ytest, s = "lambda.min")["mse"]
#> $mse
#> lambda.min
#>   10.99374
#> attr(,"measure")
#> [1] "Mean-Squared Error"

without.pretraining =  cv.glmnet(x, y, family = "gaussian", type.measure = "mse",
                                 foldid = train.folds)

# Prediction squared error without pretraining:
assess.glmnet(without.pretraining, xtest, newy = ytest, s = "lambda.min")["mse"]
#> $mse
#> lambda.min
#>   14.78239
#> attr(,"measure")
#> [1] "Mean-Squared Error"
```

References

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