Executable Jupyter notebook 2: Medical data for regression

In [1]:

```
# imports and plotting utility functions
%matplotlib inline
import warnings

import numpy as np
from scipy.linalg import norm
import pandas as pd

from sklearn.datasets import make_regression
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error
from sklearn.ensemble import RandomForestRegressor
from sklearn.cross_validation import ShuffleSplit
from sklearn.linear_model import Lasso
from statsmodels.regression.linear_model import OLS

from matplotlib import pylab as plt
import seaborn as sns

warnings.filterwarnings('ignore')

rf_cmp = RandomForestRegressor(n_estimators=250, criterion='mse', bootstrap=True
, oob_score=True, random_state=0)

def plot_lr(true_coefs, est_coefs, pvals, var_names=None, rf_cmp_coef=None):
    n_feat = len(est_coefs)
    where_sign = lr_pvalues < 0.05
    plt.figure(figsize=(15, 7))
    # print non-significant betas
    plt.scatter(np.arange(X.shape[1]), est_coefs, s=150, color='red', label='est
imated betas', alpha=0.5)
    if true_coefs is not None:
        plt.scatter(np.arange(X.shape[1]), true_coefs, s=150, color='black', lab
el='true betas', alpha=0.5)
    if rf_cmp_coef is not None:
        plt.scatter(np.arange(X.shape[1]), rf_cmp_coef, s=150, marker='D', color
='steelblue', label='RandomForest importances', alpha=0.5)

    # print star significant betas and their values
    axes = plt.gca()
    #import pdb; pdb.set_trace()
    y_min, y_max = axes.get_ylim()
    axes.set_ylim(y_min * 1.25, y_max * 1.25)
    sign_y = np.sum(where_sign) * [y_min]
    plt.scatter(np.arange(X.shape[1])[where_sign], sign_y, color='red', label='s
ignificant at p<0.05', s=150, marker=(5, 1), alpha=0.75, linewidth=3)
    for i_b, p in enumerate(pvals):
        plt.text(x=i_b - 0.25, y=y_min * 1.10, s='$p$=%.3f' % p)

    plt.xlabel('input variables')
    #plt.xticks(np.arange(n_feat)[::2], (np.arange(n_feat) + 1)[::2])
    if var_names is None:
        plt.xticks(np.arange(n_feat), (np.arange(n_feat) + 1), fontsize=16)
    else:
        plt.xticks(np.arange(n_feat), var_names, fontsize=16)
    plt.grid(True)
    plt.title('Linear regression', fontsize=16)
    plt.legend(loc='upper right', fontsize=14, fancybox=True, framealpha=0.5)
```

```python
def plot_regr_paths(coefs, accs, nonzeros, C_grid, var_names=None, unbiased_accs
=None, metric=None):
    n_cols = 2
    n_rows = 1
    n_verticals = len(coefs)
    n_feat = coefs.shape[1]

    my_palette = np.array([
        '#F47D7D', '#FBEF69', '#98E466', '#000000',
        '#A7794F', '#CCCCCC', '#85359C', '#FF9300', '#FF0030', 'grey', 'blue',
'salmon', '#4BBCF6',
        'green', 'tomato', 'darkred', 'black', 'cyan', 'lime'
    ])
    my_colors = np.array(['???????'] * coefs.shape[-1])
    i_col = 0
    new_grp_pts_x = []
    new_grp_pts_y = []
    new_grp_pts_col = []
    new_grp_pts_total = []

    for i_vertical, (params, acc, C) in enumerate(zip(
        coefs, accs, C_grid)):
        b_notset = my_colors == '???????'
        b_nonzeros = params == 0
        b_coefs_of_new_grp = np.logical_and(b_notset, b_nonzeros)

        #if i_vertical >= 17:
        #    import pdb; pdb.set_trace()

        if np.sum(b_coefs_of_new_grp) > 0:
            i_col += 1

            # we found a new subset that became 0
            for new_i in np.where(b_coefs_of_new_grp == True)[0]:
                # color all coefficients of the current group
                cur_col = my_palette[i_col]
                my_colors[new_i] = cur_col

            new_grp_pts_x.append(C)
            new_grp_pts_y.append(acc)
            new_grp_pts_col.append(cur_col)
            new_grp_pts_total.append(np.sum(b_nonzeros))

    if var_names is None:
        X_colnames = np.arange(n_feat) + 1
    else:
        X_colnames = var_names

    subplot_xlabel = '#nonzero coefficients'

    f, axarr = plt.subplots(nrows=n_rows, ncols=n_cols,
        figsize=(15, 10), facecolor='white')
    t, i_col = 0, 0

    for i_line in range(X.shape[-1]):
        axarr[i_col].plot(np.log10(C_grid),
            coefs[:, i_line], label=X_colnames[i_line],
                color=my_colors[i_line], linewidth=1.5)

    # axarr[0].set_xticks(np.arange(len(C_grid)))
    # axarr[0].set_xticklabels(np.log10(C_grid))  #, rotation=75)
    axarr[i_col].set_xlabel(subplot_xlabel, fontsize=10)
    axarr[i_col].legend(loc='lower left', fontsize=11, markerscale=10, fancybox=
True, framealpha=0.5)
    axarr[0].grid(True)
    # axarr[i_col].set_ylabel('Item groups', fontsize=16)
    axarr[0].set_title('LASSO: Groups of selected variables', fontsize=16)
    axarr[0].set_xticks(np.log10(C_grid))
    axarr[0].set_xticklabels(nonzeros)

    # axarr[1].axis('off')
    #import pdb; pdb.set_trace()
    axarr[1].grid(True)
    if unbiased_accs is not None:
        axarr[1].scatter(np.arange(len(unbiased_accs)), unbiased_accs, color='or
ange',
                     linewidth=4, label='prediction accuracy (unbiased)', zorder
=10)
    axarr[1].scatter(np.arange(len(accs)), accs, color='black',
                     linewidth=3, label='prediction accuracy', zorder=10)
    # axarr[1].set_title('ACCURACY')
    if metric == mean_absolute_error:
        error_title = 'LASSO: Out-of-sample performance (MAD score)'
    else:
        axarr[1].set_ylim(-0.15, 1.05)
        error_title = 'LASSO: Out-of-sample performance ($R^2$ score)'
    # axarr[1].set_xticklabels(np.log10(C_grid), '')
    axarr[1].set_xticks(np.arange(n_verticals))
    axarr[1].set_xticklabels(nonzeros)
    axarr[1].set_xlabel(subplot_xlabel, fontsize=10)
    # axarr[1].set_ylabel('Out-of-sample performance', fontsize=16)
    axarr[1].legend(loc='lower left', fontsize=14, markerscale=1, fancybox=True,
 framealpha=0.5)
    axarr[1].set_title(error_title, fontsize=16)
    return my_colors

def corrfunc(x, y, **kws):
    from scipy import stats
    r, _ = stats.pearsonr(x, y)
    ax = plt.gca()
    ax.annotate("r = {:.2f}".format(r),
                xy=(.1, .9), xycoords=ax.transAxes)
```

```
/Users/dengeman/anaconda3/lib/python3.5/site-packages/sklearn/cross_
validation.py:41: DeprecationWarning: This module was deprecated in
version 0.18 in favor of the model_selection module into which all t
he refactored classes and functions are moved. Also note that the in
terface of the new CV iterators are different from that of this modu
le. This module will be removed in 0.20.
  "This module will be removed in 0.20.", DeprecationWarning)
```

In [2]:

```
import statsmodels.api as sm

# https://datascience.stackexchange.com/questions/937/does-scikit-learn-have-for
ward-selection-stepwise-regression-algorithm
def fwd_stepwise_selection(X, y, initial_list=[], verbose=True):
    """ Perform a forward-backward feature selection
    based on p-value from statsmodels.api.OLS
    Arguments:
        X - pandas.DataFrame with candidate features
        y - list-like with the target
        initial_list - list of features to start with (column names of X)
        threshold_in - include a feature if its p-value < threshold_in
        threshold_out - exclude a feature if its p-value > threshold_out
        verbose - whether to print the sequence of inclusions and exclusions
    Returns: list of selected features
    """
    included = list(initial_list)
    while len(included) < X.shape[1]:
        # forward step
        excluded = list(set(X.columns)-set(included))
        new_pval = pd.Series(index=excluded)
        for new_column in excluded:
            model = sm.OLS(y, sm.add_constant(pd.DataFrame(X[included + [new_col
umn]]))).fit()
            new_pval[new_column] = model.pvalues[new_column]
        best_pval = new_pval.min()
        best_feature = new_pval.argmin()
        included.append(best_feature)
        if verbose:
            print('Add  {:30} with p-value {:.6}'.format(best_feature, best_pval
))
    return included
```

In [3]:

```
# statistical helper functions
def compute_Lasso_regpath(X, y, C_grid, metric=None, verbose=True):
    coef_list2 = []
    acc_list2 = []
    acc_unbiased_list2 = []
    nonzero_list2 = []
    if metric is None:
        metric = r2_score
    for i_step, my_C in enumerate(C_grid):
        sample_accs = []
        sample_accs_unbiased = []
        sample_coef = []
        for i_subsample in range(100):
            folder = ShuffleSplit(n=len(y), n_iter=100, test_size=0.1,
                                  random_state=i_subsample)
            train_inds, test_inds = next(iter(folder))

            clf = Lasso(alpha=my_C, random_state=i_subsample)

            clf.fit(X[train_inds, :], y[train_inds])
            acc = metric(
                    y_true=y[test_inds],
                    y_pred=clf.predict(X[test_inds]))

            # get out-of-sample accuracy from unbiased linear model with selecte
d inputs
            b_vars_to_keep = clf.coef_ != 0
            if np.sum(b_vars_to_keep) > 0:
                unbiased_lr = LinearRegression()
                unbiased_lr.fit(
                  X[train_inds, :][:, b_vars_to_keep], y[train_inds])
                unbiased_acc = metric(
                    y_true=y[test_inds],
                    y_pred=unbiased_lr.predict(X[test_inds][:, b_vars_to_keep]))
            else:
                unbiased_acc = 0

            sample_accs.append(acc)
            sample_accs_unbiased.append(unbiased_acc)
            sample_coef.append(clf.coef_)

        mean_coefs = np.mean(np.array(sample_coef), axis=0)
        coef_list2.append(mean_coefs)
        acc_for_C = np.mean(sample_accs)
        acc_for_C_unbaised = np.mean(sample_accs_unbiased)
        acc_list2.append(acc_for_C)
        acc_unbiased_list2.append(np.mean(sample_accs_unbiased))
        notzero = np.count_nonzero(mean_coefs)
        nonzero_list2.append(notzero)
        if verbose:
            print("alpha: %.4f acc: %.2f / %.2f (unbiased) active_coefs: %i" % (
                my_C, acc_for_C, acc_for_C_unbaised, notzero))
    return np.array(coef_list2), np.array(acc_list2), np.array(nonzero_list2), n
p.array(acc_unbiased_list2)
```

In [4]:

```
def infpred_plot(unbiased_acc_list, lr_pvalues, coef_list, feat_names, acc_offse
t=0.1, annot_ha='center'):
    fig = plt.figure(figsize=(9, 9))
    sorter = unbiased_acc_list.argsort()[::-1]
    colors = plt.cm.viridis_r(np.linspace(0.1, 0.9, len(sorter)))

    unique_nonzero = {}
    size = 20
    for ii, idx in enumerate(sorter):
        acc = unbiased_acc_list[idx]
        non_zero = np.where(coef_list[idx])[0]
        if tuple(non_zero) not in unique_nonzero:
            unique_nonzero[tuple(non_zero)] = non_zero
        else:
            print('skipping', ii)
            continue

        xx = -np.log10(lr_pvalues[non_zero])
        this_acc = np.array([acc] * len(xx))
        size *= 0.9
        plt.plot(xx + np.random.sample(len(xx)) * 0.01,
                 this_acc,
                 marker='o', linestyle='None',
                 color=colors[ii], zorder=-ii,
                 alpha=0.9,
                 mfc='None',
                 mew=1,
                 markersize=size)
        if ii == 0:
            psorter = np.argsort(lr_pvalues)
            feat_names_ = [feat_names[kk] for kk in psorter]
            xx2 = -np.log10(lr_pvalues[psorter])
            for jj, (this_name, this_x) in enumerate(zip(feat_names_, xx2)):
                print(this_x)
                plt.annotate(
                    this_name, xy=(this_x, acc + acc_offset),
                    xycoords='data', rotation=90,
                    verticalalignment='bottom' if jj % 2 else 'top',
                    ha=annot_ha,
                    fontsize=14)
    plt.axvline(
        -np.log10(0.05), color='red', linestyle='--', linewidth=3)
    plt.annotate('p < 0.05', xy=(-np.log10(0.045), 0.03), color='red', fontsize=
16)
    plt.xlabel(r'significance [$-log_{10}(p)$]', fontsize=20, fontweight=150)
    plt.ylabel(r'prediction [$R^2$]', fontsize=20, fontweight=150)
    plt.ylim(0, 1)
    plt.grid(True)
    ax = plt.gca()
    ax.set_yticks([0., 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1])
    ax.set_yticks(np.arange(0.01, 1, 0.01), minor=True);
    return fig
```

Diabetes: 2 very predictive, but only 1 significant variable

Dataset summary: Ten baseline variables, age, sex, body mass index, average blood pressure, and six blood serum measurements were obtained for each of n = 442 diabetes patients, as well as the response of interest, a quantitative measure of disease progression one year after baseline.

Data Set Characteristics:

:Number of Instances: 442

:Number of Attributes: First 10 columns are numeric predictive values

:Target: Column 11 is a quantitative measure of disease progression one year after baseline

:Attributes: :Age: :Sex: :Body mass index: :Average blood pressure: :S1: :S2: :S3: :S4: :S5: :S6:

Note: Each of these 10 feature variables have been mean centered and scaled by the standard deviation times `n_samples` (i.e. the sum of squares of each column totals 1).

Source URL: http://www4.stat.ncsu.edu/~boos/var.select/diabetes.html (http://www4.stat.ncsu.edu/~boos/var.select/diabetes.html)

For more information see: Bradley Efron, Trevor Hastie, Iain Johnstone and Robert Tibshirani (2004) "Least Angle Regression," Annals of Statistics (with discussion), 407-499. (http://web.stanford.edu/~hastie/Papers/LARS/LeastAngle_2002.pdf (http://web.stanford.edu/~hastie/Papers/LARS/LeastAngle_2002.pdf))

In [5]:

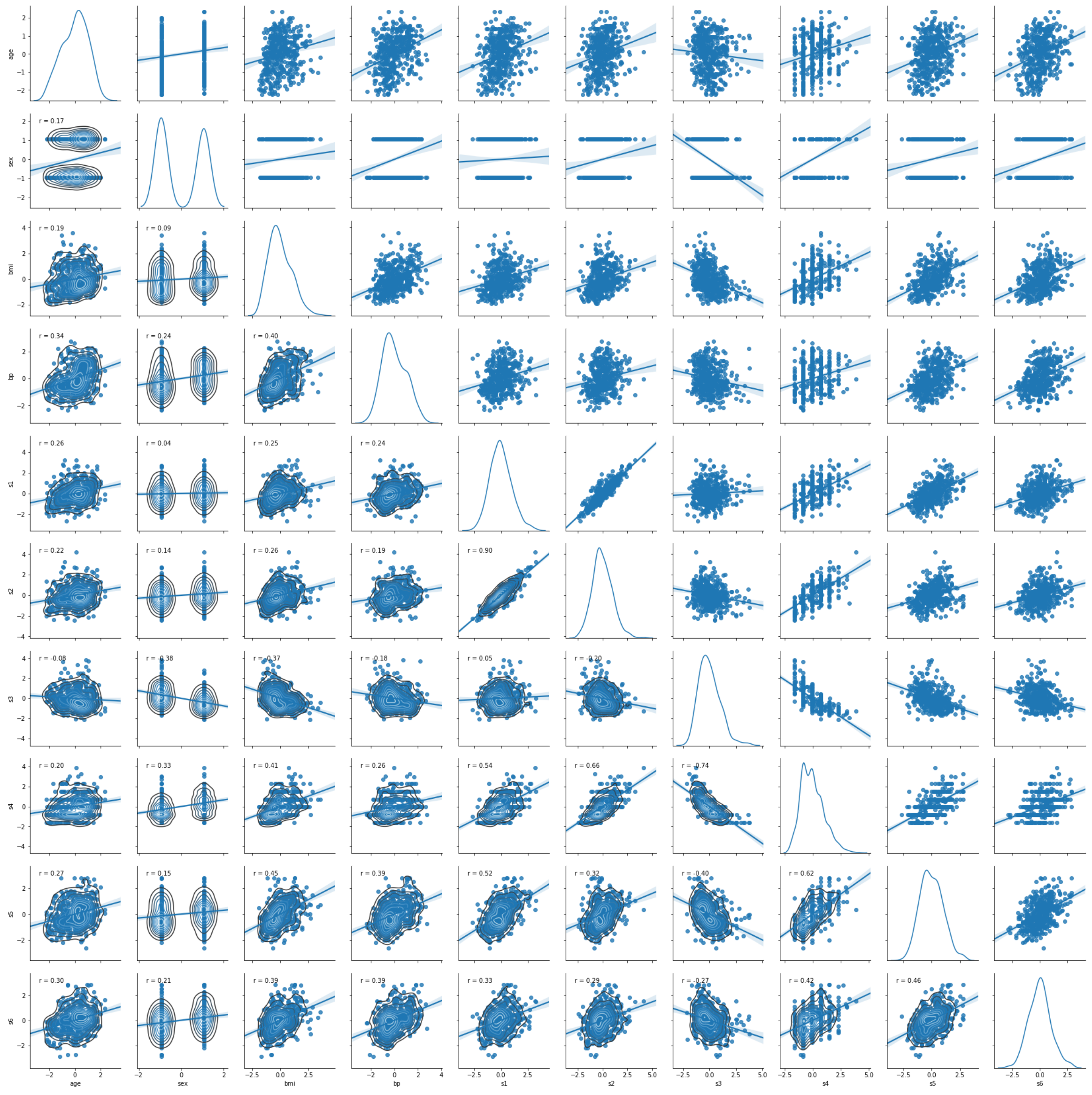
```
import sklearn.datasets as ds
bun = ds.load_diabetes()
X, y = bun.data, bun.target
X = StandardScaler().fit_transform(X)
feat_names = bun.feature_names
```

In [6]:

```
g = sns.pairplot(pd.DataFrame(X, columns=feat_names), kind="reg", diag_kind="kd
e")
g.map_lower(sns.kdeplot, cmap="Blues_d")
g.map_lower(corrfunc)
```

Out[6]:

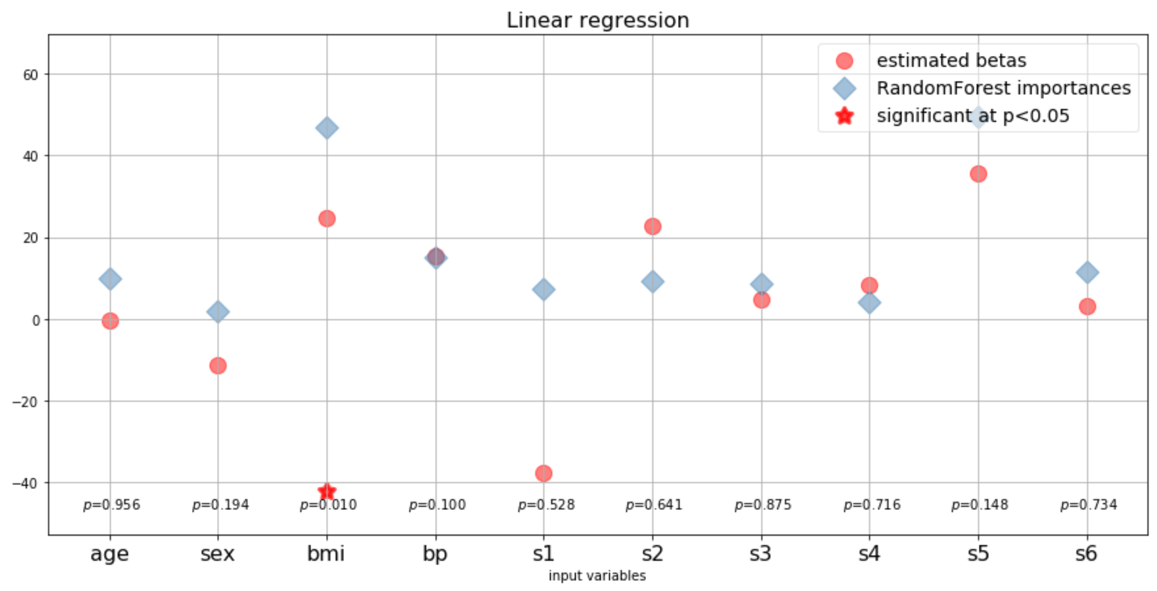
```
<seaborn.axisgrid.PairGrid at 0x127db7278>
```

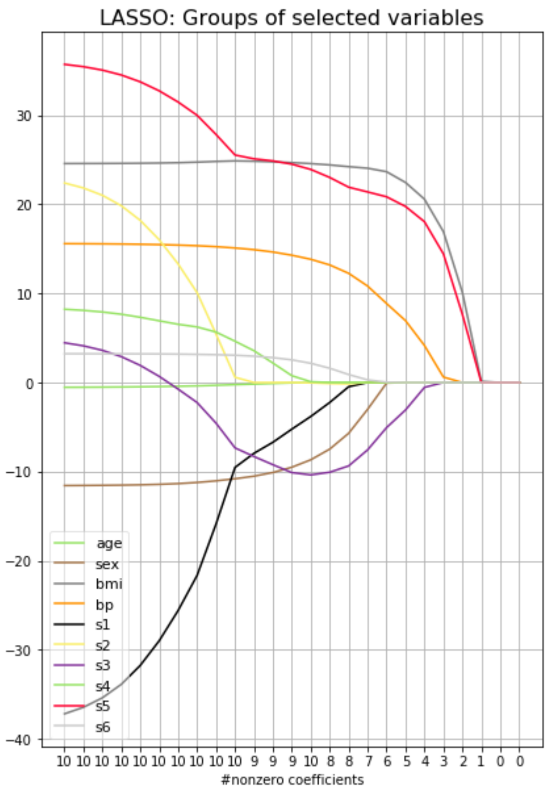


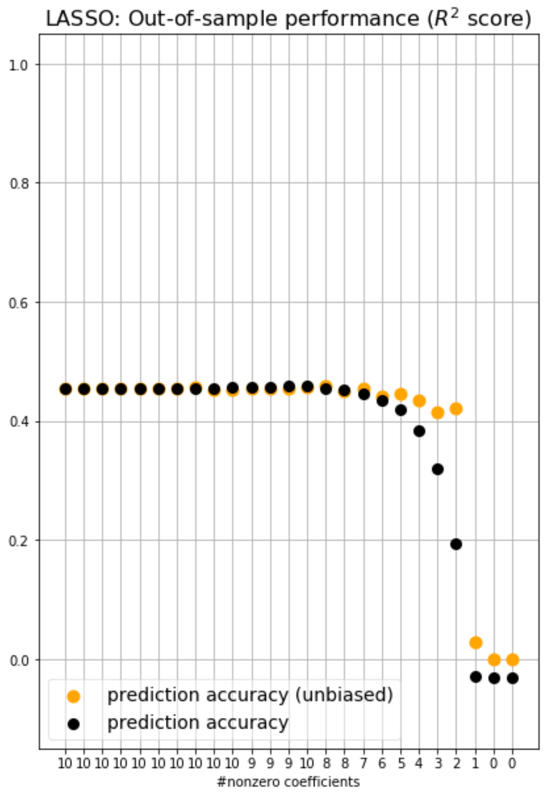
In [7]:

```
# ordinary least squares
model = OLS(y, X)
res = model.fit()
lr_coefs = res.params
lr_pvalues = res.pvalues

snr = (norm(a=lr_coefs, ord=2) ** 2) / (norm(a=res.resid, ord=2) ** 2)
print('Signal-to-noise ratio: %.4f' % snr)

rf_cmp.fit(X, y)
rf_cmp.feature_importances_

# compute Lasso regularization paths
C_grid = np.logspace(-2, 2, 25)
coef_list, acc_list, nonzero_list, unbiased_acc_list = compute_Lasso_regpath(X,
y, C_grid)

plot_lr(None, lr_coefs, lr_pvalues, feat_names, rf_cmp_coef=rf_cmp.feature_impor
tances_ * 10 * np.mean(np.abs(lr_coefs)))
path_colors = plot_regr_paths(coef_list, acc_list, nonzero_list, C_grid, feat_na
mes, unbiased_acc_list)
```

```
Signal-to-noise ratio: 0.0004
alpha: 0.0100 acc: 0.45 / 0.45 (unbiased) active_coefs: 10
alpha: 0.0147 acc: 0.45 / 0.45 (unbiased) active_coefs: 10
alpha: 0.0215 acc: 0.45 / 0.45 (unbiased) active_coefs: 10
alpha: 0.0316 acc: 0.45 / 0.45 (unbiased) active_coefs: 10
alpha: 0.0464 acc: 0.45 / 0.45 (unbiased) active_coefs: 10
alpha: 0.0681 acc: 0.45 / 0.45 (unbiased) active_coefs: 10
alpha: 0.1000 acc: 0.46 / 0.45 (unbiased) active_coefs: 10
alpha: 0.1468 acc: 0.46 / 0.46 (unbiased) active_coefs: 10
alpha: 0.2154 acc: 0.46 / 0.45 (unbiased) active_coefs: 10
alpha: 0.3162 acc: 0.46 / 0.45 (unbiased) active_coefs: 10
alpha: 0.4642 acc: 0.46 / 0.46 (unbiased) active_coefs: 9
alpha: 0.6813 acc: 0.46 / 0.45 (unbiased) active_coefs: 9
alpha: 1.0000 acc: 0.46 / 0.45 (unbiased) active_coefs: 9
alpha: 1.4678 acc: 0.46 / 0.46 (unbiased) active_coefs: 10
alpha: 2.1544 acc: 0.46 / 0.46 (unbiased) active_coefs: 8
alpha: 3.1623 acc: 0.45 / 0.45 (unbiased) active_coefs: 8
alpha: 4.6416 acc: 0.45 / 0.45 (unbiased) active_coefs: 7
alpha: 6.8129 acc: 0.43 / 0.44 (unbiased) active_coefs: 6
alpha: 10.0000 acc: 0.42 / 0.45 (unbiased) active_coefs: 5
alpha: 14.6780 acc: 0.38 / 0.43 (unbiased) active_coefs: 4
alpha: 21.5443 acc: 0.32 / 0.42 (unbiased) active_coefs: 3
alpha: 31.6228 acc: 0.19 / 0.42 (unbiased) active_coefs: 2
alpha: 46.4159 acc: -0.03 / 0.03 (unbiased) active_coefs: 1
alpha: 68.1292 acc: -0.03 / 0.00 (unbiased) active_coefs: 0
alpha: 100.0000 acc: -0.03 / 0.00 (unbiased) active_coefs: 0
```



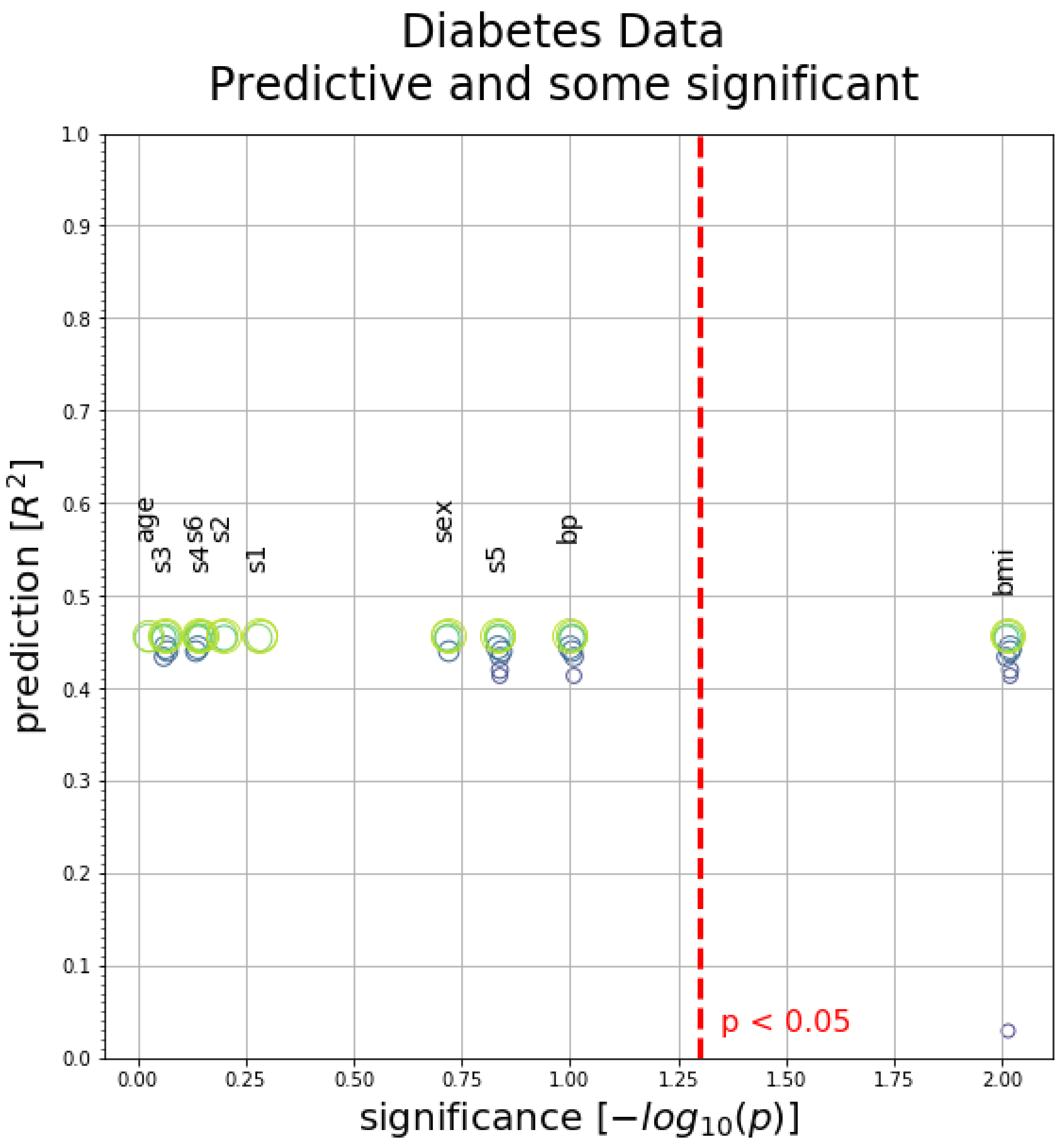

LASSO: Groups of selected variables
30
20
10
0
−10
−20
−30
−40
age
sex
bmi
bp
s1
s2
s3
s4
s5
s6
10 10 10 10 10 10 10 10 10 10 9 9 9 10 8 8 7 6 5 4 3 2 1 0 0
#nonzero coefficients


LASSO: Out-of-sample performance (R^2 score)
1.0
0.8
0.6
0.4
0.2
0.0
● prediction accuracy (unbiased)
● prediction accuracy
10 10 10 10 10 10 10 10 10 10 9 9 9 10 8 8 7 6 5 4 3 2 1 0 0
#nonzero coefficients

In [8]:

```
fig = infpred_plot(unbiased_acc_list, lr_pvalues, coef_list, feat_names)
fig.suptitle('Diabetes Data\nPredictive and some significant',
             fontsize=24, fontweight=150)
fig.savefig('reg-case1.pdf', bbox_inches='tight')
```

```
2.00836758255
0.99805835067
0.831173523726
0.711931965772
0.277160066083
0.193251734924
0.145088838637
0.134406512913
0.0581639211354
0.0196968809084
skipping 2
skipping 4
skipping 5
skipping 7
skipping 8
skipping 9
skipping 10
skipping 11
skipping 12
skipping 13
skipping 14
skipping 15
skipping 16
skipping 24
```

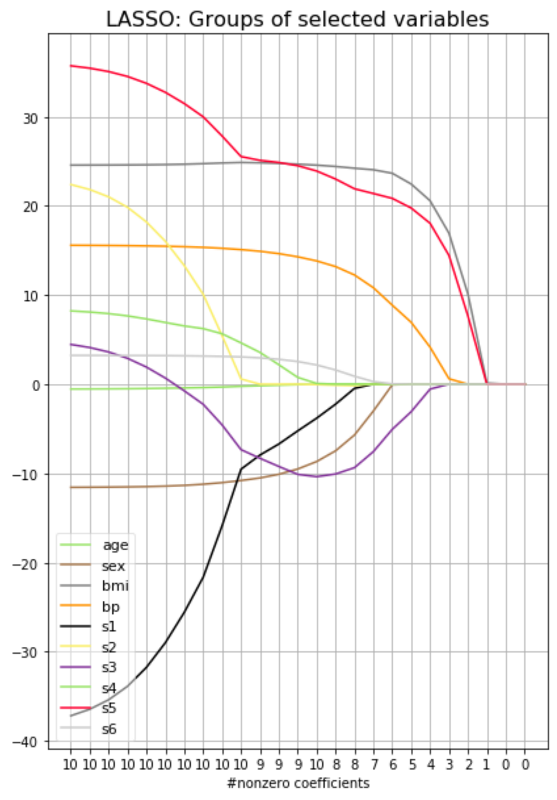

Diabetes Data
Predictive and some significant
prediction [R^2]
significance [$-log_{10}(p)$]
p < 0.05
age
s3
s4
s6
s2
s1
sex
s5
bp
bmi
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00

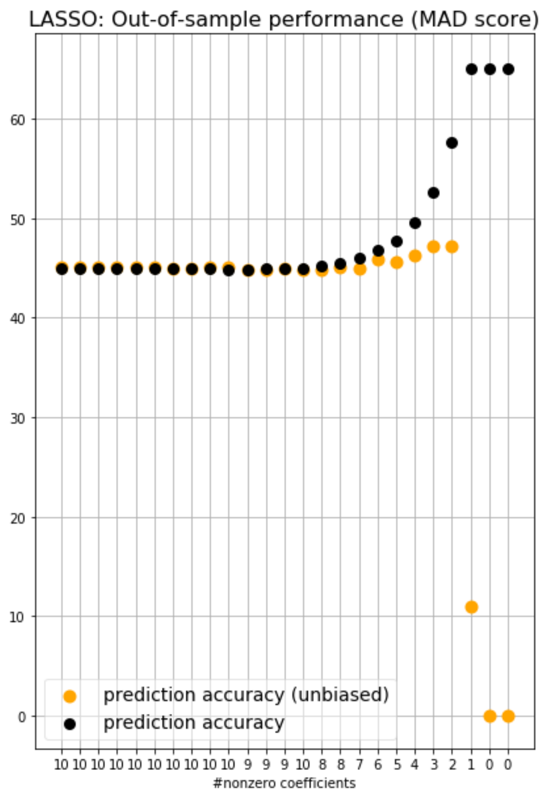
In [9]:

```
C_grid = np.logspace(-2, 2, 25)
coef_list, acc_list, nonzero_list, unbiased_acc_list = compute_Lasso_regpath(X,
y, C_grid, metric=mean_absolute_error, verbose=False)
plot_regr_paths(coef_list, acc_list, nonzero_list, C_grid, feat_names, unbiased_
acc_list, metric=mean_absolute_error)
```

Out[9]:

```
array(['#98E466', '#A7794F', 'grey', '#FF9300', '#000000', '#FBEF6
9',
       '#85359C', '#98E466', '#FF0030', '#CCCCCC'],
      dtype='<U7')
```





In [10]:

```
sel_w_pvals = fwd_stepwise_selection(pd.DataFrame(X, columns=feat_names), y, ver
bose=True)
print('Forward-stepwise selection: ' +  ' -> '.join(sel_w_pvals))
```

```
Add  bmi                            with p-value 3.46601e-42
Add  s5                             with p-value 3.03968e-20
Add  bp                             with p-value 3.74192e-05
Add  s1                             with p-value 0.00145437
Add  sex                            with p-value 0.00922919
Add  s2                             with p-value 0.000272264
Add  s4                             with p-value 0.261918
Add  s6                             with p-value 0.304022
Add  s3                             with p-value 0.638562
Add  age                            with p-value 0.867
Forward-stepwise selection: bmi -> s5 -> bp -> s1 -> sex -> s2 -> s4
-> s6 -> s3 -> age
```

conclusions

- only var 3 significant, prediction: this one is selected too but as predictive as var 9 and similar to 4 and 7 -> S5 is as predictive as bmi but not significant, same goes for bp and s3
- bp has a lower p-value than s5, but s5 is nevertheless more predictive than bp (partly explained by their correlation of 0.39)
- bmi is significant, but alone R2 is less 0.05 !!!!!!!!!!!!!
- some of the most correlated input variables are neither significant nor predictive

```
In [11]:
```

```
res.summary(xname=feat_names)
```

```
Out[11]:
```

OLS Regression Results

Dep. Variable:	y	**R-squared:**	0.106
Model:	OLS	**Adj. R-squared:**	0.085
Method:	Least Squares	**F-statistic:**	5.100
Date:	Sun, 20 May 2018	**Prob (F-statistic):**	4.72e-07
Time:	17:29:08	**Log-Likelihood:**	-2873.9
No. Observations:	442	**AIC:**	5768.
Df Residuals:	432	**BIC:**	5809.
Df Model:	10		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
age	-0.4762	8.560	-0.056	0.956	-17.301	16.348
sex	-11.4070	8.771	-1.301	0.194	-28.647	5.832
bmi	24.7263	9.532	2.594	0.010	5.991	43.461
bp	15.4297	9.373	1.646	0.100	-2.992	33.852
s1	-37.6804	59.697	-0.631	0.528	-155.014	79.653
s2	22.6765	48.573	0.467	0.641	-72.792	118.145
s3	4.8062	30.449	0.158	0.875	-55.041	64.653
s4	8.4221	23.134	0.364	0.716	-37.048	53.892
s5	35.7347	24.628	1.451	0.148	-12.671	84.140
s6	3.2166	9.453	0.340	0.734	-15.364	21.797

Omnibus:	1.506	**Durbin-Watson:**	0.223
Prob(Omnibus):	0.471	**Jarque-Bera (JB):**	1.404
Skew:	0.017	**Prob(JB):**	0.496
Kurtosis:	2.726	**Cond. No.**	21.7

Prostata dataset: not significant, but predictive

Prostate Cancer Data Description These data come from a study that examined the correlation between the level of prostate specific antigen and a number of clinical measures in men who were about to receive a radical prostatectomy. It is data frame with 97 rows and 9 columns.

Usage data(Prostate) Format The data frame has the following components:

lcavol log(cancer volume) lweight log(prostate weight) age age lbph log(benign prostatic hyperplasia amount) svi seminal vesicle invasion lcp log(capsular penetration) gleason Gleason score pgg45 percentage Gleason scores 4 or 5 lpsa log(prostate specific antigen) Source Stamey, T.A., Kabalin, J.N., McNeal, J.E., Johnstone, I.M., Freiha, F., Redwine, E.A. and Yang, N. (1989) Prostate specific antigen in the diagnosis and treatment of adenocarcinoma of the prostate: II. radical prostatectomy treated patients, Journal of Urology 141(5), 1076–1083.

Lasso paths from Hastie et al. 2001

image.png

In [12]:

```
import pandas as pd
df_prostate = pd.read_csv('dataset_prostate.csv')
y = df_prostate['lpsa']
feat_names = ['lcavol', 'lweight', 'age', 'lbph', 'svi', 'lcp', 'gleason', 'pgg4
5']
X = StandardScaler().fit_transform(df_prostate[feat_names])
```

In [13]:

```
df_prostate
```

Out[13]:

	Unnamed: 0	lcavol	lweight	age	lbph	svi	lcp	gleason	pgg45	
0	1	-0.579818	2.769459	50	-1.386294	0	-1.386294	6	0	-0.
1	2	-0.994252	3.319626	58	-1.386294	0	-1.386294	6	0	-0.
2	3	-0.510826	2.691243	74	-1.386294	0	-1.386294	7	20	-0.
3	4	-1.203973	3.282789	58	-1.386294	0	-1.386294	6	0	-0.
4	5	0.751416	3.432373	62	-1.386294	0	-1.386294	6	0	0.3
5	6	-1.049822	3.228826	50	-1.386294	0	-1.386294	6	0	0.7
6	7	0.737164	3.473518	64	0.615186	0	-1.386294	6	0	0.7
7	8	0.693147	3.539509	58	1.536867	0	-1.386294	6	0	0.8
8	9	-0.776529	3.539509	47	-1.386294	0	-1.386294	6	0	1.0
9	10	0.223144	3.244544	63	-1.386294	0	-1.386294	6	0	1.0
10	11	0.254642	3.604138	65	-1.386294	0	-1.386294	6	0	1.2
11	12	-1.347074	3.598681	63	1.266948	0	-1.386294	6	0	1.2
12	13	1.613430	3.022861	63	-1.386294	0	-0.597837	7	30	1.2
13	14	1.477049	2.998229	67	-1.386294	0	-1.386294	7	5	1.3
14	15	1.205971	3.442019	57	-1.386294	0	-0.430783	7	5	1.3
15	16	1.541159	3.061052	66	-1.386294	0	-1.386294	6	0	1.4
16	17	-0.415515	3.516013	70	1.244155	0	-0.597837	7	30	1.4
17	18	2.288486	3.649359	66	-1.386294	0	0.371564	6	0	1.4
18	19	-0.562119	3.267666	41	-1.386294	0	-1.386294	6	0	1.5
19	20	0.182322	3.825375	70	1.658228	0	-1.386294	6	0	1.5
20	21	1.147402	3.419365	59	-1.386294	0	-1.386294	6	0	1.6
21	22	2.059239	3.501043	60	1.474763	0	1.348073	7	20	1.6
22	23	-0.544727	3.375880	59	-0.798508	0	-1.386294	6	0	1.6
23	24	1.781709	3.451574	63	0.438255	0	1.178655	7	60	1.7
24	25	0.385262	3.667400	69	1.599388	0	-1.386294	6	0	1.7
25	26	1.446919	3.124565	68	0.300105	0	-1.386294	6	0	1.7
26	27	0.512824	3.719651	65	-1.386294	0	-0.798508	7	70	1.8
27	28	-0.400478	3.865979	67	1.816452	0	-1.386294	7	20	1.8
28	29	1.040277	3.128951	67	0.223144	0	0.048790	7	80	1.8
29	30	2.409644	3.375880	65	-1.386294	0	1.619388	6	0	1.8
...	...	...	...	...	...	...	...	...	...	...
67	68	2.198335	4.050915	72	2.307573	0	-0.430783	7	10	2.9

	Unnamed: 0	lcavol	lweight	age	lbph	svi	lcp	gleason	pgg45	
68	69	-0.446287	4.408547	69	-1.386294	0	-1.386294	6	0	2.9
69	70	1.193922	4.780383	72	2.326302	0	-0.798508	7	5	2.9
70	71	1.864080	3.593194	60	-1.386294	1	1.321756	7	60	3.0
71	72	1.160021	3.341093	77	1.749200	0	-1.386294	7	25	3.0
72	73	1.214913	3.825375	69	-1.386294	1	0.223144	7	20	3.0
73	74	1.838961	3.236716	60	0.438255	1	1.178655	9	90	3.0
74	75	2.999226	3.849083	69	-1.386294	1	1.909543	7	20	3.2
75	76	3.141130	3.263849	68	-0.051293	1	2.420368	7	50	3.3
76	77	2.010895	4.433789	72	2.122262	0	0.500775	7	60	3.3
77	78	2.537657	4.354784	78	2.326302	0	-1.386294	7	10	3.4
78	79	2.648300	3.582129	69	-1.386294	1	2.583998	7	70	3.4
79	80	2.779440	3.823192	63	-1.386294	0	0.371564	7	50	3.5
80	81	1.467874	3.070376	66	0.559616	0	0.223144	7	40	3.5
81	82	2.513656	3.473518	57	0.438255	0	2.327278	7	60	3.5
82	83	2.613007	3.888754	77	-0.527633	1	0.559616	7	30	3.5
83	84	2.677591	3.838376	65	1.115142	0	1.749200	9	70	3.5
84	85	1.562346	3.709907	60	1.695616	0	0.810930	7	30	3.5
85	86	3.302849	3.518980	64	-1.386294	1	2.327278	7	60	3.6
86	87	2.024193	3.731699	58	1.638997	0	-1.386294	6	0	3.6
87	88	1.731656	3.369018	62	-1.386294	1	0.300105	7	30	3.7
88	89	2.807594	4.718052	65	-1.386294	1	2.463853	7	60	3.9
89	90	1.562346	3.695110	76	0.936093	1	0.810930	7	75	3.9
90	91	3.246491	4.101817	68	-1.386294	0	-1.386294	6	0	4.0
91	92	2.532903	3.677566	61	1.348073	1	-1.386294	7	15	4.1
92	93	2.830268	3.876396	68	-1.386294	1	1.321756	7	60	4.3
93	94	3.821004	3.896909	44	-1.386294	1	2.169054	7	40	4.6
94	95	2.907447	3.396185	52	-1.386294	1	2.463853	7	10	5.1
95	96	2.882564	3.773910	68	1.558145	1	1.558145	7	80	5.4
96	97	3.471966	3.974998	68	0.438255	1	2.904165	7	20	5.5

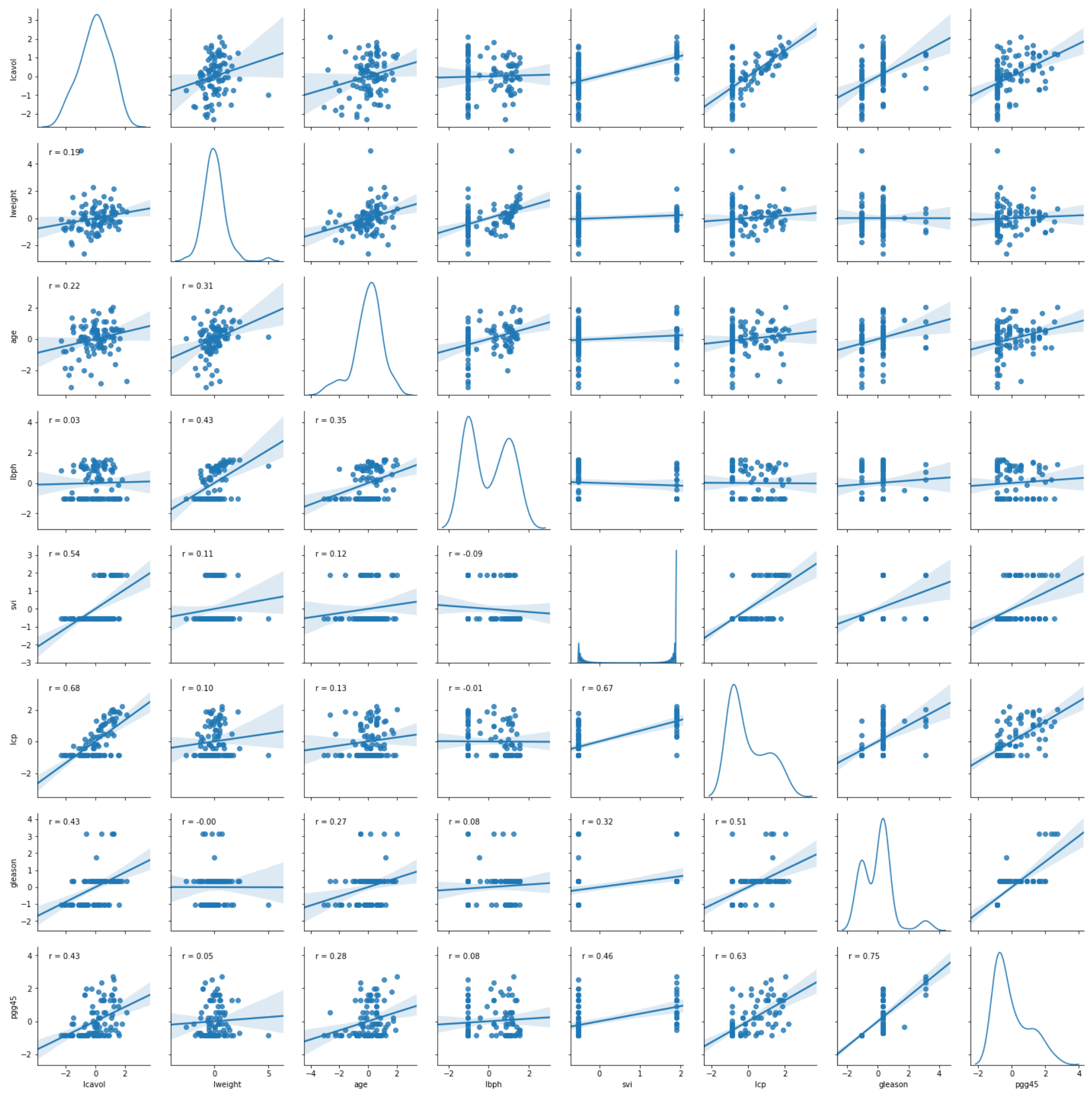
97 rows × 10 columns

In [14]:

```
g = sns.pairplot(pd.DataFrame(X, columns=feat_names), kind="reg", diag_kind="kd
e")
g.map_lower(corrfunc)
```

Out[14]:

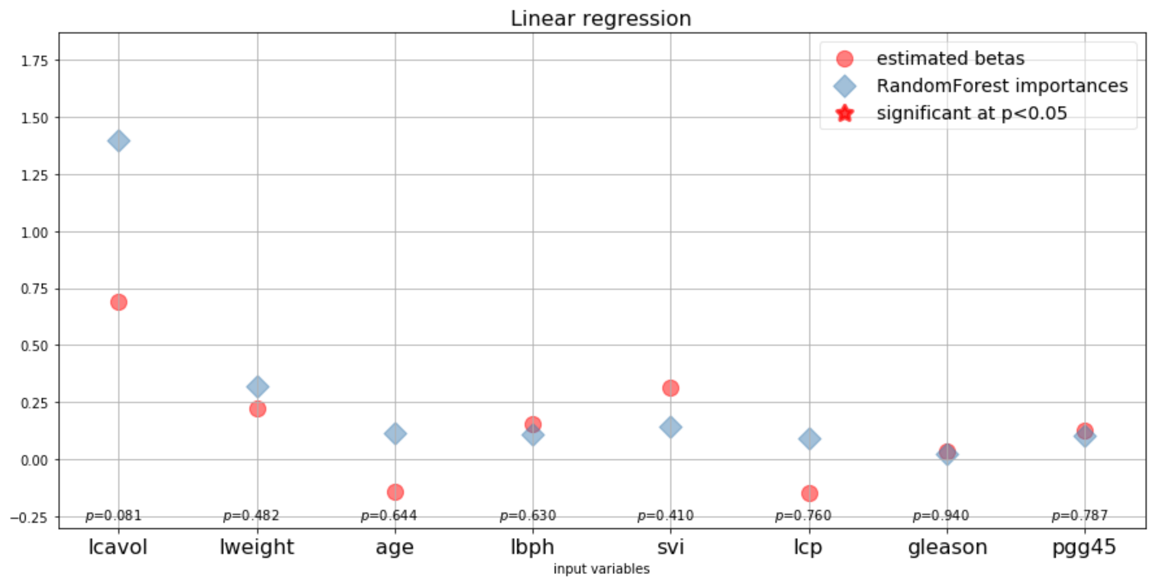
```
<seaborn.axisgrid.PairGrid at 0x130a7bb38>
```

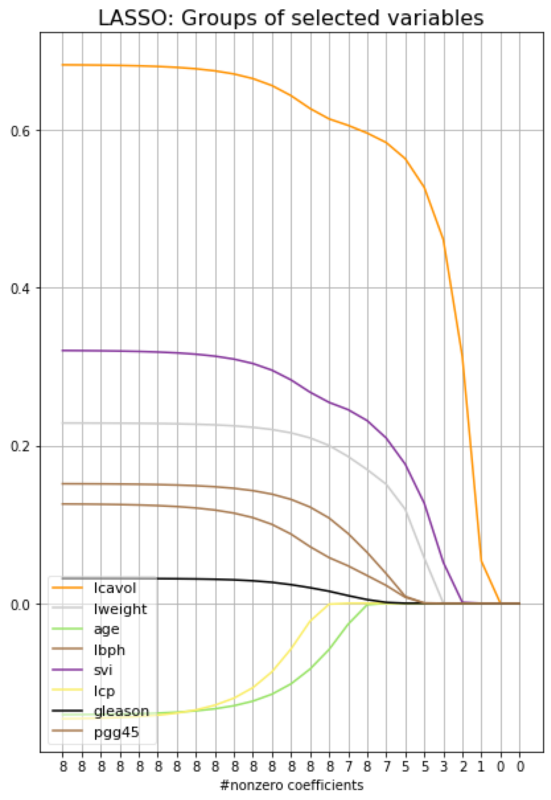


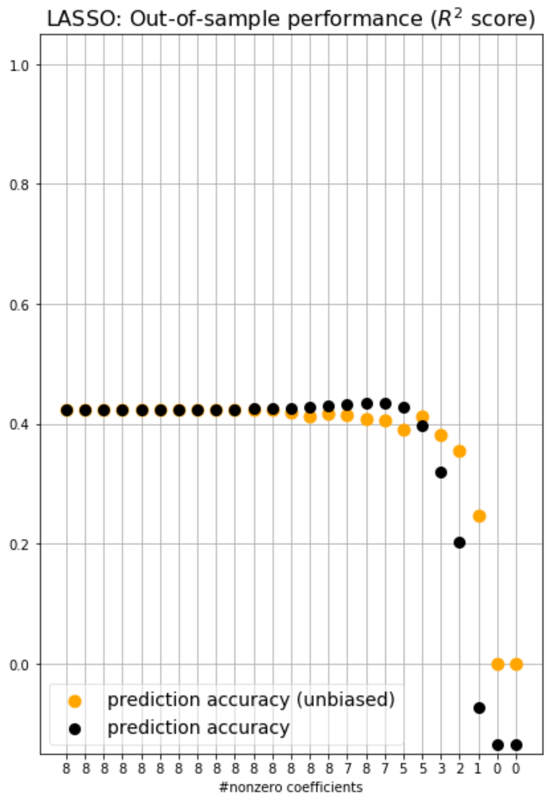
In [15]:

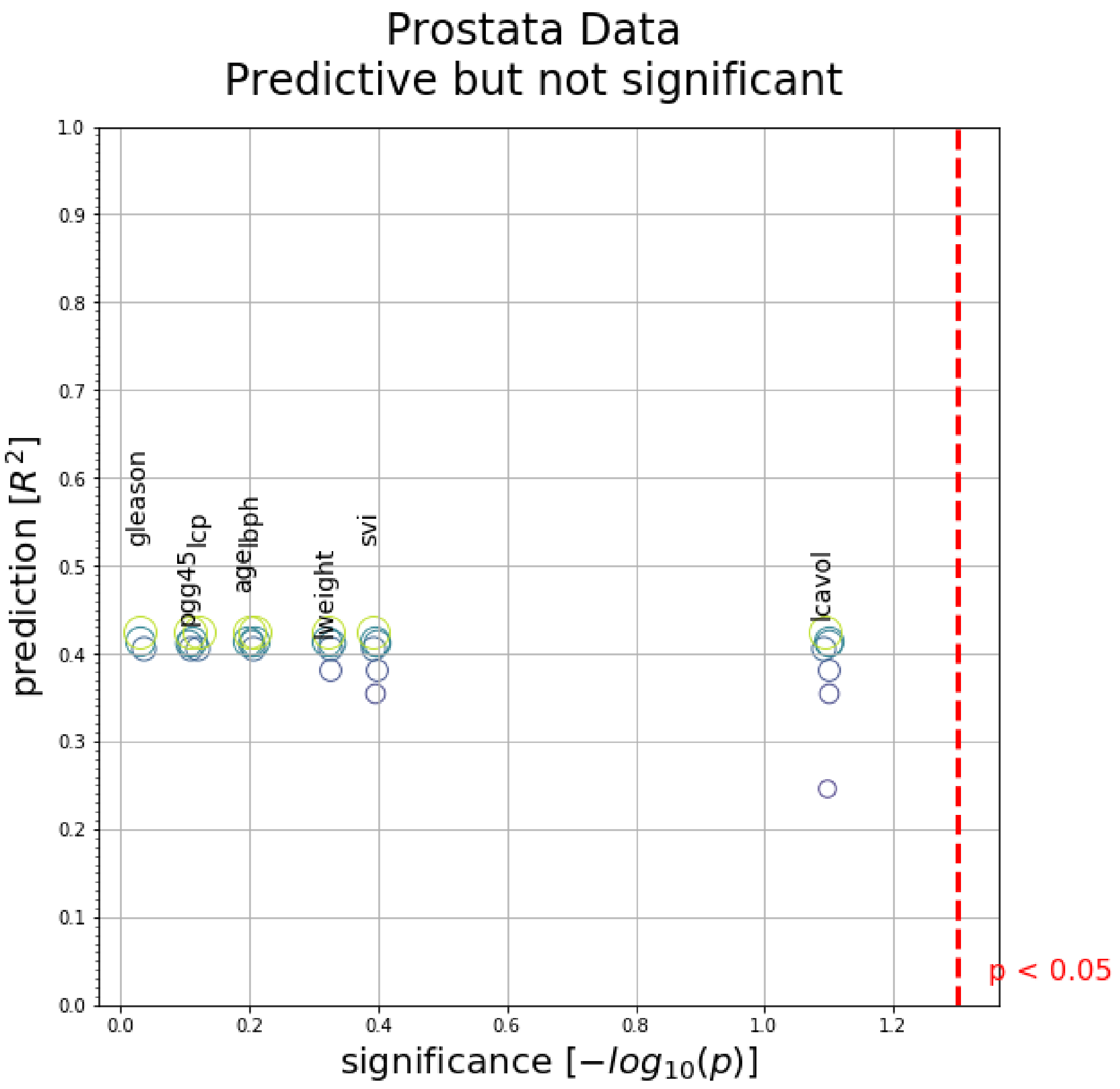
```
# ordinary least squares
model = OLS(y, X)
res = model.fit()
lr_coefs = res.params
lr_pvalues = res.pvalues

snr = (norm(a=lr_coefs, ord=2) ** 2) / (norm(a=res.resid, ord=2) ** 2)
print('Signal-to-noise ratio: %.4f' % snr)

rf_cmp.fit(X, y)
rf_cmp.feature_importances_

# compute Lasso regularization paths
C_grid = np.logspace(-4, 0.25, 25)
coef_list, acc_list, nonzero_list, unbiased_acc_list = compute_Lasso_regpath(X,
y, C_grid)

plot_lr(None, lr_coefs, lr_pvalues, feat_names, rf_cmp_coef=rf_cmp.feature_impor
tances_ * 10 * np.mean(np.abs(lr_coefs)))
plot_regr_paths(coef_list, acc_list, nonzero_list, C_grid, feat_names, unbiased_
acc_list)


fig = infpred_plot(unbiased_acc_list, lr_pvalues, coef_list, feat_names)
fig.suptitle('Prostata Data\nPredictive but not significant',
             fontsize=24, fontweight=150)
fig.savefig('reg-case2.pdf', bbox_inches='tight')
```

```
Signal-to-noise ratio: 0.0011
alpha: 0.0001 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0002 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0002 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0003 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0005 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0008 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0012 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0017 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0026 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0039 acc: 0.42 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0059 acc: 0.43 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0089 acc: 0.43 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0133 acc: 0.43 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0200 acc: 0.43 / 0.41 (unbiased) active_coefs: 8
alpha: 0.0301 acc: 0.43 / 0.42 (unbiased) active_coefs: 8
alpha: 0.0453 acc: 0.43 / 0.41 (unbiased) active_coefs: 7
alpha: 0.0681 acc: 0.44 / 0.41 (unbiased) active_coefs: 8
alpha: 0.1024 acc: 0.44 / 0.41 (unbiased) active_coefs: 7
alpha: 0.1540 acc: 0.43 / 0.39 (unbiased) active_coefs: 5
alpha: 0.2315 acc: 0.40 / 0.41 (unbiased) active_coefs: 5
alpha: 0.3481 acc: 0.32 / 0.38 (unbiased) active_coefs: 3
alpha: 0.5233 acc: 0.20 / 0.35 (unbiased) active_coefs: 2
alpha: 0.7867 acc: -0.07 / 0.25 (unbiased) active_coefs: 1
alpha: 1.1828 acc: -0.14 / 0.00 (unbiased) active_coefs: 0
alpha: 1.7783 acc: -0.14 / 0.00 (unbiased) active_coefs: 0
1.09052420155
0.387620170856
0.31702692195
0.20088814274
0.191418331703
0.119070652787
0.10376282393
0.0269610992509
skipping 1
skipping 2
skipping 3
skipping 4
skipping 5
skipping 6
skipping 7
skipping 8
skipping 9
skipping 10
skipping 11
skipping 12
skipping 13
skipping 16
skipping 17
skipping 19
skipping 24
```


Linear regression
estimated betas
RandomForest importances
significant at p<0.05
p=0.081
p=0.482
p=0.644
p=0.630
p=0.410
p=0.760
p=0.940
p=0.787
lcavol
lweight
age
lbph
svi
lcp
gleason
pgg45
input variables


LASSO: Groups of selected variables
lcavol
lweight
age
lbph
svi
lcp
gleason
pgg45
#nonzero coefficients


LASSO: Out-of-sample performance (R^2 score)
prediction accuracy (unbiased)
prediction accuracy
#nonzero coefficients



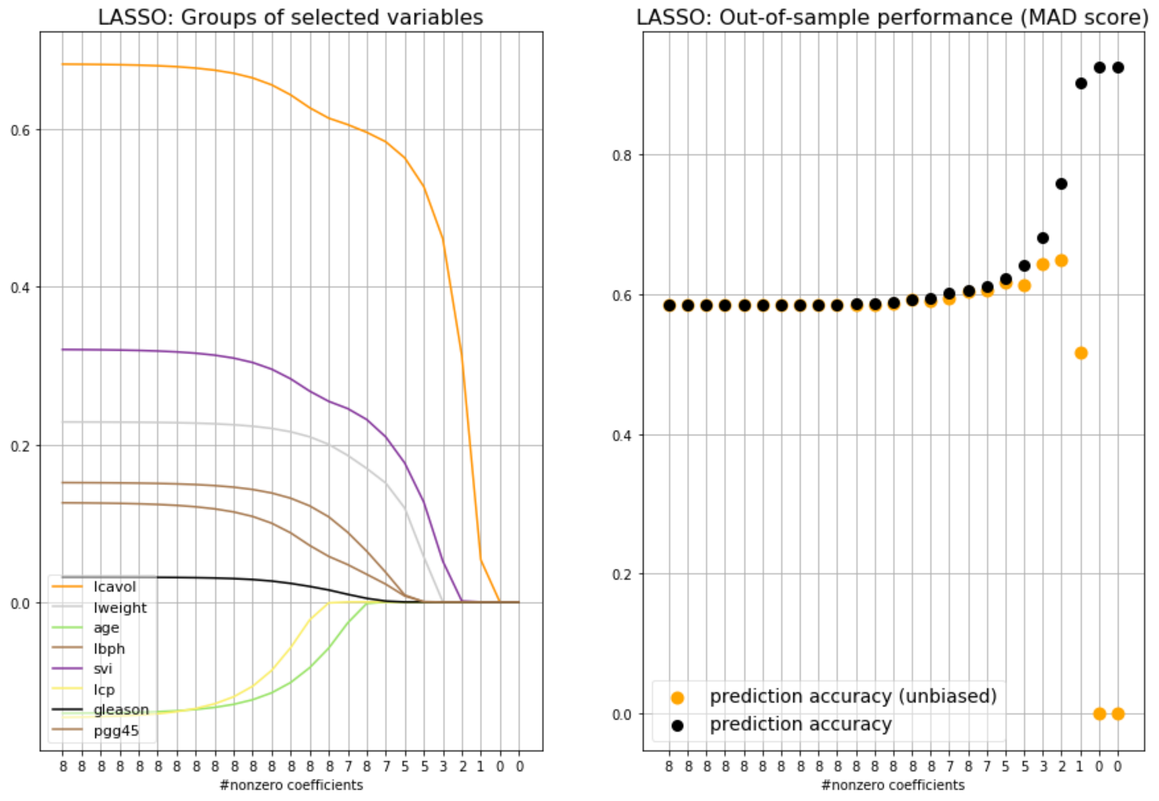
Prostata Data
Predictive but not significant
prediction [R^2]
significance [$-log_{10}(p)$]
gleason
pgg45
lcp
age
lbph
lweight
svi
lcavol
p < 0.05
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2

In [16]:

```
C_grid = np.logspace(-4, 0.25, 25)
coef_list, acc_list, nonzero_list, unbiased_acc_list = compute_Lasso_regpath(X,
y, C_grid, metric=mean_absolute_error, verbose=False)
plot_regr_paths(coef_list, acc_list, nonzero_list, C_grid, feat_names, unbiased_
acc_list, metric=mean_absolute_error)
```

Out[16]:

```
array(['#FF9300', '#CCCCCC', '#98E466', '#A7794F', '#85359C', '#FBEF
69',
       '#000000', '#A7794F'],
      dtype='<U7')
```



In [17]:

```
sel_w_pvals = fwd_stepwise_selection(pd.DataFrame(X, columns=feat_names), y, ver
bose=True)
print('Forward-stepwise selection: ' + ' -> '.join(sel_w_pvals))
```

```
Add  lcavol                            with p-value 1.11861e-17
Add  lweight                           with p-value 0.00160649
Add  svi                               with p-value 0.00202903
Add  lbph                              with p-value 0.11213
Add  age                               with p-value 0.169527
Add  pgg45                             with p-value 0.253309
Add  lcp                               with p-value 0.251271
Add  gleason                           with p-value 0.77506
Forward-stepwise selection: lcavol -> lweight -> svi -> lbph -> age
-> pgg45 -> lcp -> gleason
```

conclusions:

- no significants (trending significant at 0.08 is also single most predictive variable)
- ~5 items not full set of 9 variables were clearly very predictive -> the widely practiced Gleason score (?) comes up as disturbing prediction
- second-most important variable diverged in fwd-stepwise selection and Lasso selection -> tiny difference

In [18]:

```
res.summary(xname=feat_names)
```

Out[18]:

OLS Regression Results

Dep. Variable:	lpsa	**R-squared:**	0.116
Model:	OLS	**Adj. R-squared:**	0.036
Method:	Least Squares	**F-statistic:**	1.456
Date:	Sun, 20 May 2018	**Prob (F-statistic):**	0.185
Time:	17:29:40	**Log-Likelihood:**	-229.14
No. Observations:	97	**AIC:**	474.3
Df Residuals:	89	**BIC:**	494.9
Df Model:	8		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
lcavol	0.6883	0.390	1.764	0.081	-0.087	1.464
lweight	0.2245	0.318	0.706	0.482	-0.407	0.856
age	-0.1454	0.313	-0.464	0.644	-0.768	0.477
lbph	0.1545	0.319	0.484	0.630	-0.480	0.789
svi	0.3155	0.381	0.828	0.410	-0.441	1.072
lcp	-0.1467	0.479	-0.306	0.760	-1.099	0.805
gleason	0.0324	0.428	0.076	0.940	-0.818	0.883
pgg45	0.1270	0.470	0.270	0.787	-0.806	1.060

Omnibus:	0.235	**Durbin-Watson:**	0.104
Prob(Omnibus):	0.889	**Jarque-Bera (JB):**	0.026
Skew:	-0.017	**Prob(JB):**	0.987
Kurtosis:	3.073	**Cond. No.**	4.12

FEV: significant but largely ignorable for prediction

In [19]:

```
import pandas as pd
df_fev = pd.read_csv('dataset_FEV.csv')

df_fev.drop(labels='id', axis=1, inplace=True)
```

In [20]:

```
df_fev
```

```
Out[20]:
```

	age	fev	height	sex	smoke
0	9	1.708	57.0	female	non-current smoker
1	8	1.724	67.5	female	non-current smoker
2	7	1.720	54.5	female	non-current smoker
3	9	1.558	53.0	male	non-current smoker
4	9	1.895	57.0	male	non-current smoker
5	8	2.336	61.0	female	non-current smoker
6	6	1.919	58.0	female	non-current smoker
7	6	1.415	56.0	female	non-current smoker
8	8	1.987	58.5	female	non-current smoker
9	9	1.942	60.0	female	non-current smoker
10	6	1.602	53.0	female	non-current smoker
11	8	1.735	54.0	male	non-current smoker
12	8	2.193	58.5	female	non-current smoker
13	8	2.118	60.5	male	non-current smoker
14	8	2.258	58.0	male	non-current smoker
15	7	1.932	53.0	male	non-current smoker
16	5	1.472	50.0	male	non-current smoker
17	6	1.878	53.0	female	non-current smoker
18	9	2.352	59.0	male	non-current smoker
19	9	2.604	61.5	male	non-current smoker
20	5	1.400	49.0	female	non-current smoker
21	5	1.256	52.5	female	non-current smoker
22	4	0.839	48.0	female	non-current smoker
23	7	2.578	62.5	male	non-current smoker
24	9	2.988	65.0	female	non-current smoker
25	3	1.404	51.5	male	non-current smoker
26	9	2.348	60.0	male	non-current smoker
27	5	1.755	52.0	male	non-current smoker
28	8	2.980	60.0	female	non-current smoker
29	9	2.100	60.0	female	non-current smoker
...	...	...	...	...	...
624	15	3.985	71.0	male	non-current smoker
625	18	4.220	68.0	male	non-current smoker

	age	fev	height	sex	smoke
626	17	4.724	70.5	male	non-current smoker
627	15	3.731	67.0	male	non-current smoker
628	17	3.406	69.0	male	current smoker
629	17	3.500	62.0	female	non-current smoker
630	16	3.674	67.5	female	non-current smoker
631	17	5.633	73.0	male	non-current smoker
632	15	3.122	64.0	female	current smoker
633	15	3.330	68.5	female	current smoker
634	16	2.608	62.0	female	current smoker
635	16	3.645	73.5	male	non-current smoker
636	15	3.799	66.5	male	current smoker
637	18	4.086	67.0	male	current smoker
638	15	2.887	63.0	female	non-current smoker
639	16	4.070	69.5	male	current smoker
640	17	3.960	70.0	male	non-current smoker
641	16	4.299	66.0	male	non-current smoker
642	16	2.981	66.0	female	non-current smoker
643	15	2.264	63.0	female	current smoker
644	18	4.404	70.5	male	current smoker
645	15	2.278	60.0	female	current smoker
646	16	4.504	72.0	male	non-current smoker
647	17	5.638	70.0	male	non-current smoker
648	16	4.872	72.0	male	current smoker
649	16	4.270	67.0	male	current smoker
650	15	3.727	68.0	male	current smoker
651	18	2.853	60.0	female	non-current smoker
652	16	2.795	63.0	female	current smoker
653	15	3.211	66.5	female	non-current smoker

654 rows × 5 columns

In [21]:

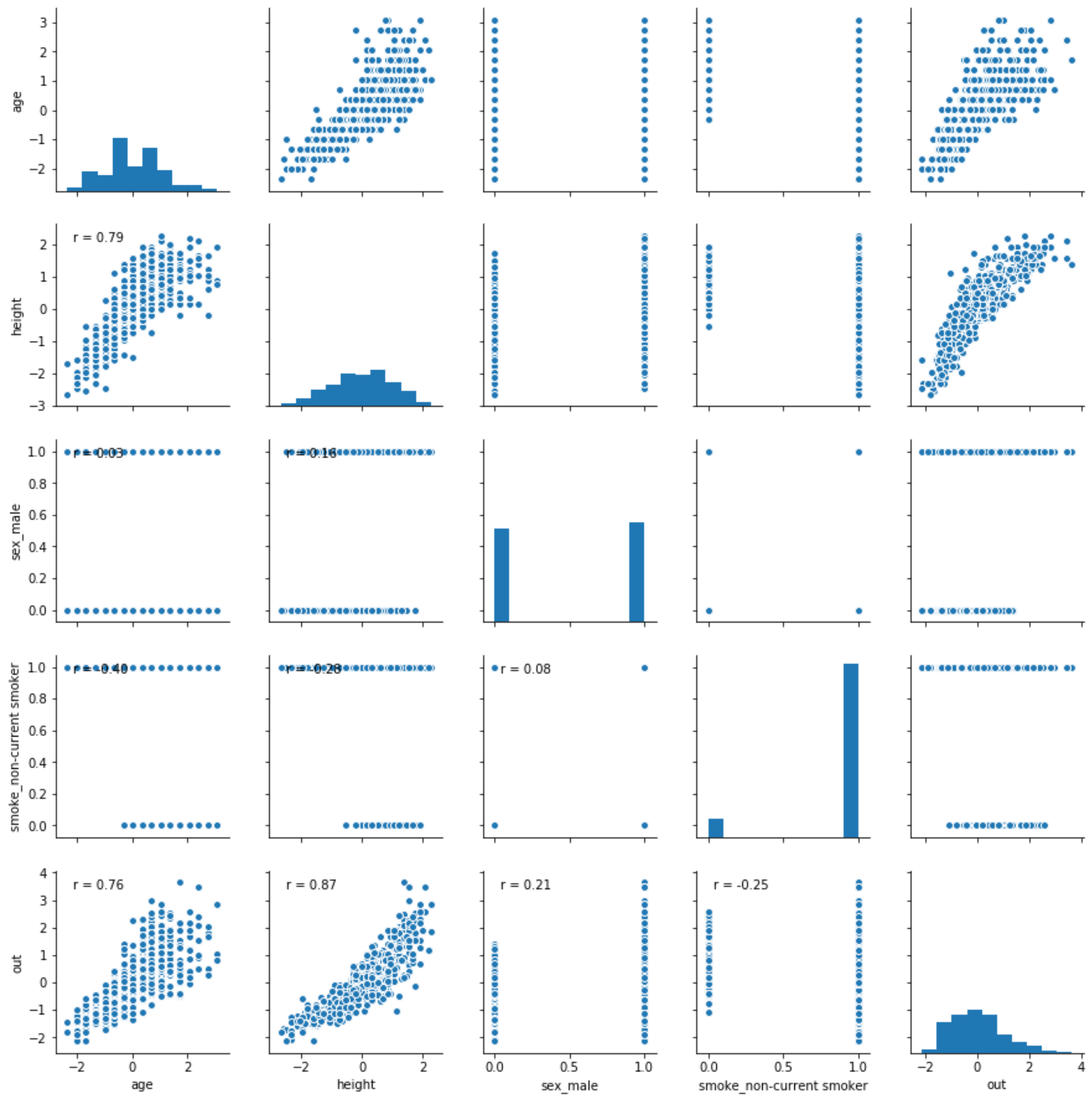
```
feat_names = ['age', u'fev', u'height', u'sex', u'smoke']
df_part1 = pd.DataFrame(StandardScaler().fit_transform(df_fev[feat_names[:-2]].v
alues), columns=feat_names[:-2])
df_part2 = pd.get_dummies(df_fev[feat_names[-2:]], drop_first=True)
#pd.concat([df_part1, df_part2], axis=1)
y = StandardScaler().fit_transform(df_part1['fev'].values[:, None])[:, 0]
df_part1.drop(labels='fev', axis=1, inplace=True)
X = np.hstack((df_part1.values, df_part2.values))
feat_names = list(df_part1.columns) + list(df_part2.columns)
```

In [22]:

```
g = sns.pairplot(pd.DataFrame(np.hstack((X, y[:, None])), columns=feat_names + [
'out']))
g.map_lower(corrfunc)
```

Out[22]:

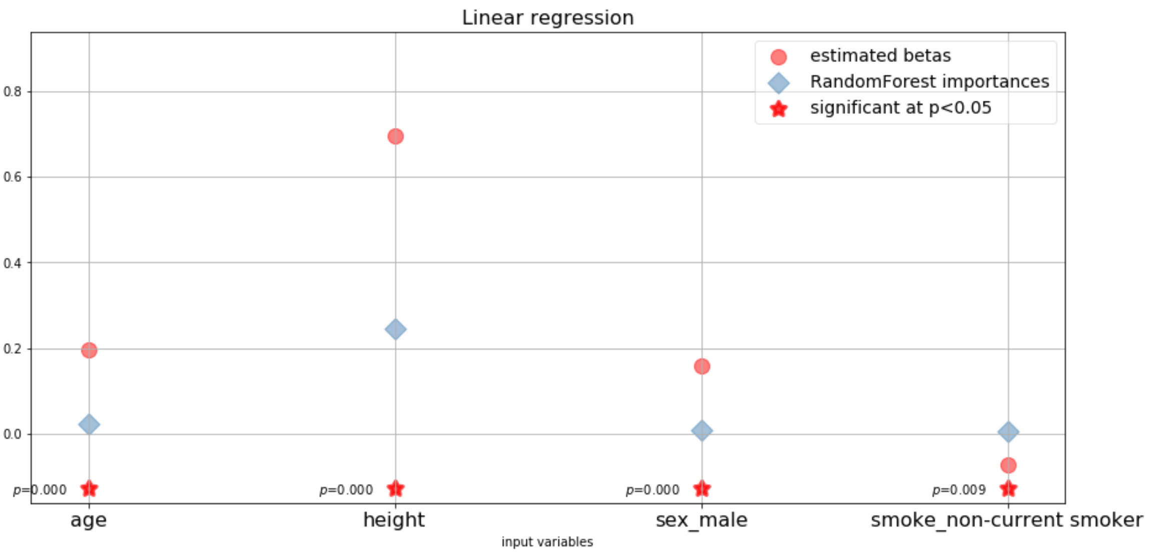
```
<seaborn.axisgrid.PairGrid at 0x12e9dad30>
```



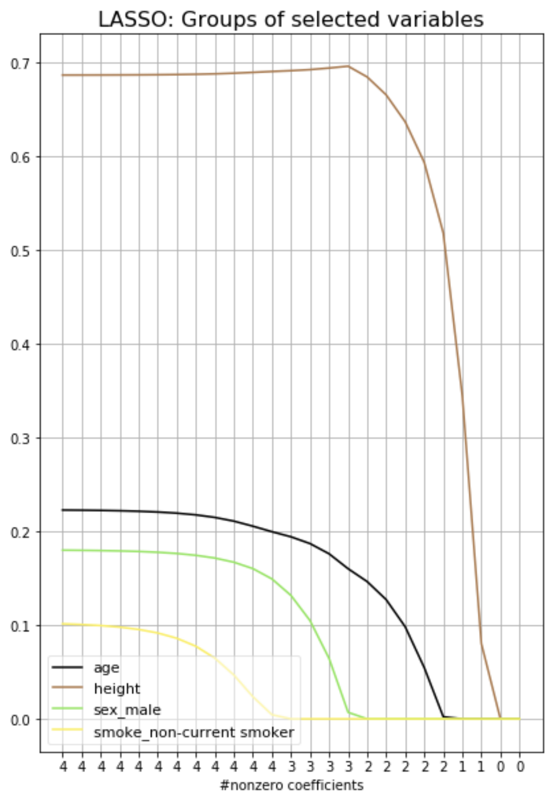
In [23]:

```
# ordinary least squares
model = OLS(y, X)
res = model.fit()
lr_coefs = res.params
lr_pvalues = res.pvalues

snr = (norm(a=lr_coefs, ord=2) ** 2) / (norm(a=res.resid, ord=2) ** 2)
print('Signal-to-noise ratio: %.4f' % snr)

rf_cmp.fit(X, y)
rf_cmp.feature_importances_

# compute Lasso regularization paths
C_grid = np.logspace(-4, 0.25, 25)
coef_list, acc_list, nonzero_list, unbiased_acc_list = compute_Lasso_regpath(X,
y, C_grid)

plot_lr(None, lr_coefs, lr_pvalues, feat_names, rf_cmp_coef=rf_cmp.feature_impor
tances_ * np.mean(np.abs(lr_coefs)))
path_colors = plot_regr_paths(coef_list, acc_list, nonzero_list, C_grid, feat_na
mes, unbiased_acc_list)

fig = infpred_plot(unbiased_acc_list, lr_pvalues, coef_list, feat_names[:-1] + [
'smoker'],
                   -0.11, annot_ha='left')
fig.suptitle('FEV Data\nsignificant but largely ignorable for prediction',
             fontsize=24, fontweight=150)
fig.savefig('reg-case3.pdf', bbox_inches='tight')
```

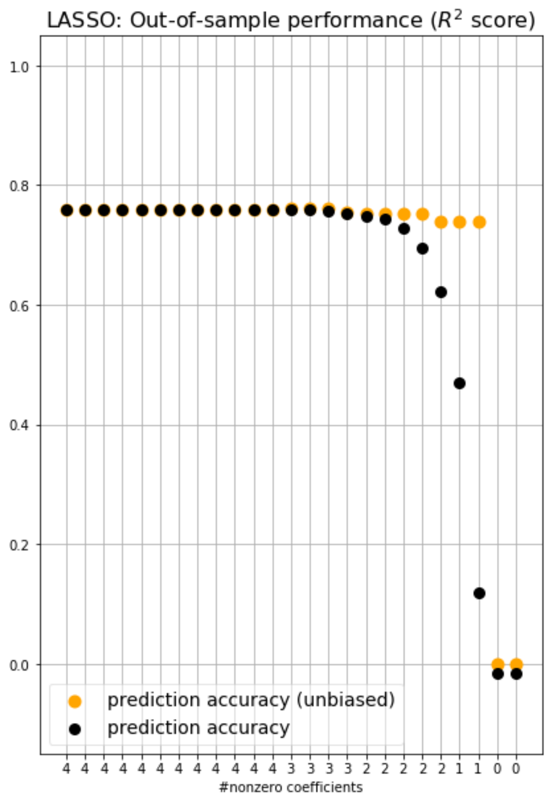
```
Signal-to-noise ratio: 0.0037
alpha: 0.0001 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0002 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0002 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0003 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0005 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0008 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0012 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0017 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0026 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0039 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0059 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0089 acc: 0.76 / 0.76 (unbiased) active_coefs: 4
alpha: 0.0133 acc: 0.76 / 0.76 (unbiased) active_coefs: 3
alpha: 0.0200 acc: 0.76 / 0.76 (unbiased) active_coefs: 3
alpha: 0.0301 acc: 0.76 / 0.76 (unbiased) active_coefs: 3
alpha: 0.0453 acc: 0.75 / 0.75 (unbiased) active_coefs: 3
alpha: 0.0681 acc: 0.75 / 0.75 (unbiased) active_coefs: 2
alpha: 0.1024 acc: 0.74 / 0.75 (unbiased) active_coefs: 2
alpha: 0.1540 acc: 0.73 / 0.75 (unbiased) active_coefs: 2
alpha: 0.2315 acc: 0.70 / 0.75 (unbiased) active_coefs: 2
alpha: 0.3481 acc: 0.62 / 0.74 (unbiased) active_coefs: 2
alpha: 0.5233 acc: 0.47 / 0.74 (unbiased) active_coefs: 1
alpha: 0.7867 acc: 0.12 / 0.74 (unbiased) active_coefs: 1
alpha: 1.1828 acc: -0.02 / 0.00 (unbiased) active_coefs: 0
alpha: 1.7783 acc: -0.02 / 0.00 (unbiased) active_coefs: 0
81.2194667249
9.29516356507
4.50372664111
2.02312839329
skipping 1
skipping 2
skipping 4
skipping 5
skipping 6
skipping 7
skipping 8
skipping 9
skipping 10
skipping 11
skipping 12
skipping 13
skipping 14
skipping 15
skipping 17
skipping 18
skipping 19
skipping 21
skipping 22
skipping 24
```



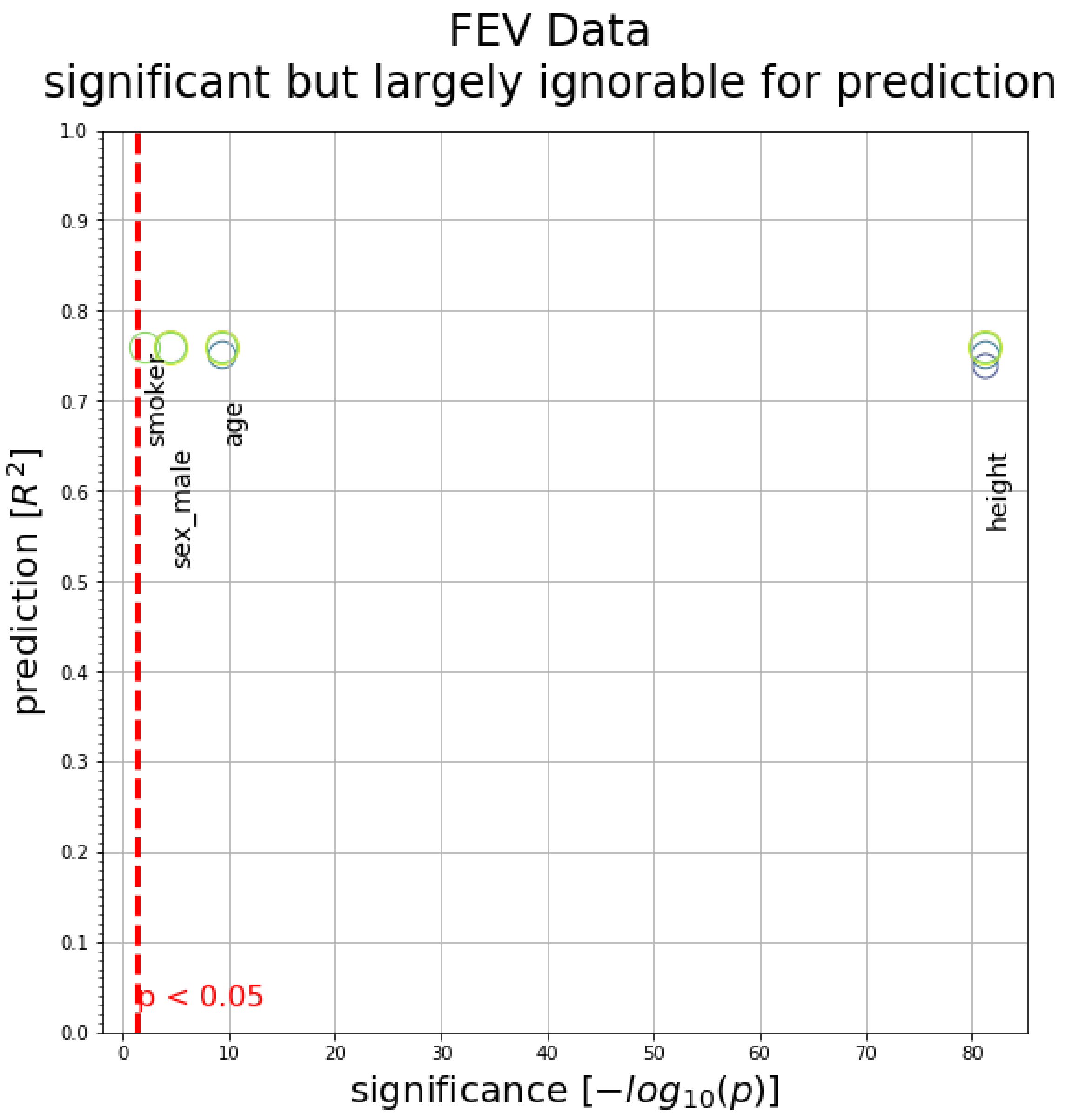
Linear regression
estimated betas
RandomForest importances
significant at p<0.05
p=0.000
p=0.000
p=0.000
p=0.009
age
height
sex_male
smoke_non-current smoker
input variables



LASSO: Groups of selected variables
age
height
sex_male
smoke_non-current smoker
#nonzero coefficients



LASSO: Out-of-sample performance (R^2 score)
prediction accuracy (unbiased)
prediction accuracy
#nonzero coefficients

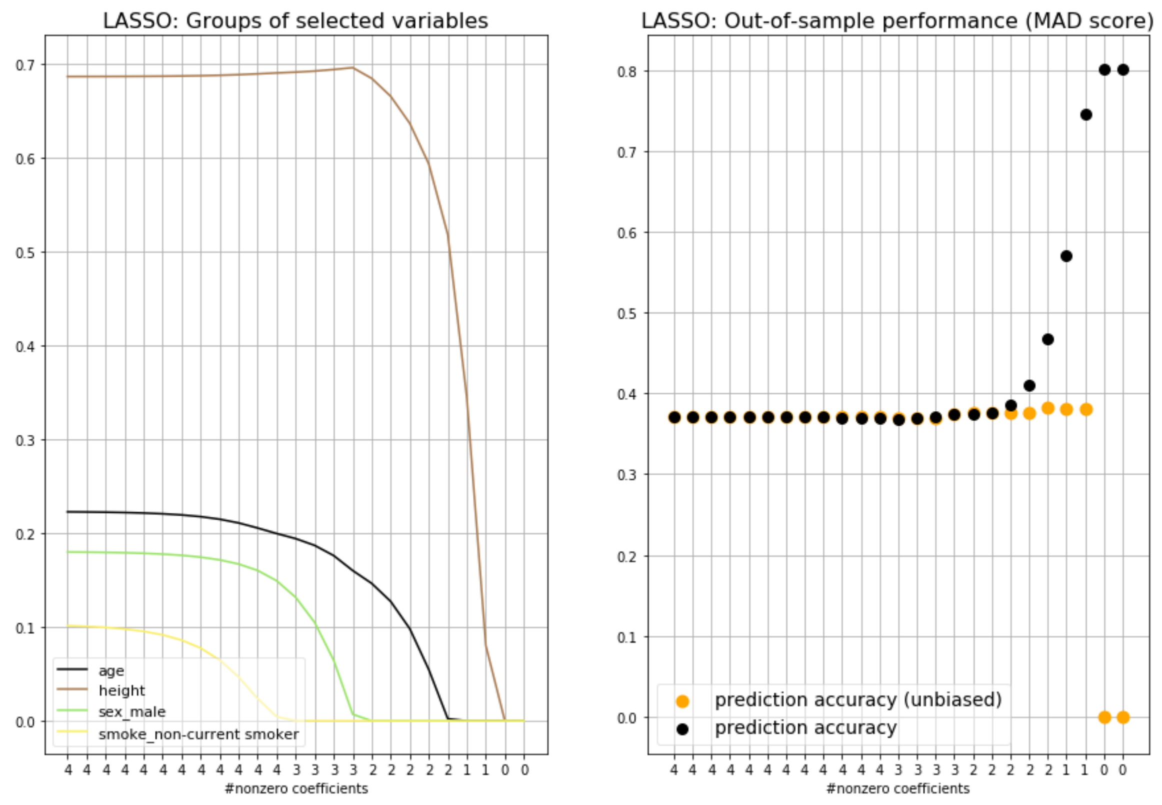

FEV Data
significant but largely ignorable for prediction
prediction [R^2]
significance [$-log_{10}(p)$]
smoker
sex_male
age
height
p < 0.05
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
10
20
30
40
50
60
70
80

In [24]:

```
C_grid = np.logspace(-4, 0.25, 25)
coef_list, acc_list, nonzero_list, unbiased_acc_list = compute_Lasso_regpath(X,
y, C_grid, metric=mean_absolute_error, verbose=False)
plot_regr_paths(coef_list, acc_list, nonzero_list, C_grid, feat_names, unbiased_
acc_list, metric=mean_absolute_error)
```

Out[24]:

```
array(['#000000', '#A7794F', '#98E466', '#FBEF69'],
      dtype='<U7')
```



In [25]:

```
sel_w_pvals = fwd_stepwise_selection(pd.DataFrame(X, columns=feat_names), y, ver
bose=True)
print('Forward-stepwise selection: ' + ' -> '.join(sel_w_pvals))
```

```
Add  height                          with p-value 1.57456e-200
Add  age                             with p-value 4.11176e-09
Add  sex_male                        with p-value 1.4463e-06
Add  smoke_non-current smoker        with p-value 0.141391
Forward-stepwise selection: height -> age -> sex_male -> smoke_non-c
urrent smoker
```

conclusions:

- 4/4 input variables are highly significant, but height alone (ignoring other 3 variables) has virtually identical accuracy in predicting FEV
- the prediction regime may miss the significant mechanistic relevance of smoking -> predictive algorithms are much more pragmatic
- high significance of all input variables is partly due to comparably high sample sizes facilitating low p values
- scientific knowledge production / scientific discovery recovers the ground truth (all 4 variables are important)
- intensive care unit: the medical doctor wants to know what to do next with the respiration machine (=prediction)

In [26]:

```
res.summary(xname=feat_names)
```

Out[26]:

OLS Regression Results

Dep. Variable:	y	**R-squared:**	0.773
Model:	OLS	**Adj. R-squared:**	0.771
Method:	Least Squares	**F-statistic:**	552.3
Date:	Sun, 20 May 2018	**Prob (F-statistic):**	2.10e-207
Time:	17:29:53	**Log-Likelihood:**	-443.60
No. Observations:	654	**AIC:**	895.2
Df Residuals:	650	**BIC:**	913.1
Df Model:	4		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
age	0.1946	0.031	6.313	0.000	0.134	0.255
height	0.6953	0.031	22.245	0.000	0.634	0.757
sex_male	0.1575	0.038	4.193	0.000	0.084	0.231
smoke_non-current smoker	-0.0735	0.028	-2.602	0.009	-0.129	-0.018

Omnibus:	25.938	**Durbin-Watson:**	1.630
Prob(Omnibus):	0.000	**Jarque-Bera (JB):**	56.330
Skew:	0.192	**Prob(JB):**	5.86e-13
Kurtosis:	4.386	**Cond. No.**	3.28

Low birth weight: significant, but hard to predict

Dataset description (R community): The birthwt data frame has 189 rows and 10 columns. The data were collected at Baystate Medical Center, Springfield, Mass during 1986.

low indicator of birth weight less than 2.5 kg.

age mother's age in years.

lwt mother's weight in pounds at last menstrual period.

race mother's race (1 = white, 2 = black, 3 = other).

smoke smoking status during pregnancy.

ptl number of previous premature labours.

ht history of hypertension.

ui presence of uterine irritability.

ftv number of physician visits during the first trimester.

bwt birth weight in grams.

Source Hosmer, D.W. and Lemeshow, S. (1989) Applied Logistic Regression. New York: Wiley

References Venables, W. N. and Ripley, B. D. (2002) Modern Applied Statistics with S. Fourth edition. Springer.

In [27]:

```
import pandas as pd
df_birth = pd.read_csv('dataset_birthwt.csv')
```

In [28]:

```
df_part1 = StandardScaler().fit_transform(df_birth[['age', 'lwt']])
df_part2 = df_birth[['race', 'smoke', 'ptl', 'ht', 'ui', 'ftv']]
#pd.concat([df_part1, df_part2], axis=1)
feat_names = ['age', 'lwt'] + list(df_part2.columns)
y = StandardScaler().fit_transform(df_birth['bwt'].values[:, None])[:, 0]
X = np.hstack((df_part1, df_part2))
```

In [29]:

```
df_birth
```

Out[29]:

	Unnamed: 0	low	age	lwt	race	smoke	ptl	ht	ui	ftv	bwt
0	85	0	19	182	2	0	0	0	1	0	2523
1	86	0	33	155	3	0	0	0	0	3	2551
2	87	0	20	105	1	1	0	0	0	1	2557
3	88	0	21	108	1	1	0	0	1	2	2594
4	89	0	18	107	1	1	0	0	1	0	2600
5	91	0	21	124	3	0	0	0	0	0	2622
6	92	0	22	118	1	0	0	0	0	1	2637
7	93	0	17	103	3	0	0	0	0	1	2637
8	94	0	29	123	1	1	0	0	0	1	2663
9	95	0	26	113	1	1	0	0	0	0	2665
10	96	0	19	95	3	0	0	0	0	0	2722
11	97	0	19	150	3	0	0	0	0	1	2733
12	98	0	22	95	3	0	0	1	0	0	2751
13	99	0	30	107	3	0	1	0	1	2	2750
14	100	0	18	100	1	1	0	0	0	0	2769
15	101	0	18	100	1	1	0	0	0	0	2769
16	102	0	15	98	2	0	0	0	0	0	2778
17	103	0	25	118	1	1	0	0	0	3	2782
18	104	0	20	120	3	0	0	0	1	0	2807
19	105	0	28	120	1	1	0	0	0	1	2821
20	106	0	32	121	3	0	0	0	0	2	2835
21	107	0	31	100	1	0	0	0	1	3	2835
22	108	0	36	202	1	0	0	0	0	1	2836
23	109	0	28	120	3	0	0	0	0	0	2863
24	111	0	25	120	3	0	0	0	1	2	2877
25	112	0	28	167	1	0	0	0	0	0	2877
26	113	0	17	122	1	1	0	0	0	0	2906
27	114	0	29	150	1	0	0	0	0	2	2920
28	115	0	26	168	2	1	0	0	0	0	2920
29	116	0	17	113	2	0	0	0	0	1	2920
...	...	...	...	...	...	...	...	...	...	...	...
159	44	1	20	80	3	1	0	0	1	0	2211
160	45	1	17	110	1	1	0	0	0	0	2225

	Unnamed: 0	low	age	lwt	race	smoke	ptl	ht	ui	ftv	bwt
161	46	1	25	105	3	0	1	0	0	1	2240
162	47	1	20	109	3	0	0	0	0	0	2240
163	49	1	18	148	3	0	0	0	0	0	2282
164	50	1	18	110	2	1	1	0	0	0	2296
165	51	1	20	121	1	1	1	0	1	0	2296
166	52	1	21	100	3	0	1	0	0	4	2301
167	54	1	26	96	3	0	0	0	0	0	2325
168	56	1	31	102	1	1	1	0	0	1	2353
169	57	1	15	110	1	0	0	0	0	0	2353
170	59	1	23	187	2	1	0	0	0	1	2367
171	60	1	20	122	2	1	0	0	0	0	2381
172	61	1	24	105	2	1	0	0	0	0	2381
173	62	1	15	115	3	0	0	0	1	0	2381
174	63	1	23	120	3	0	0	0	0	0	2410
175	65	1	30	142	1	1	1	0	0	0	2410
176	67	1	22	130	1	1	0	0	0	1	2410
177	68	1	17	120	1	1	0	0	0	3	2414
178	69	1	23	110	1	1	1	0	0	0	2424
179	71	1	17	120	2	0	0	0	0	2	2438
180	75	1	26	154	3	0	1	1	0	1	2442
181	76	1	20	105	3	0	0	0	0	3	2450
182	77	1	26	190	1	1	0	0	0	0	2466
183	78	1	14	101	3	1	1	0	0	0	2466
184	79	1	28	95	1	1	0	0	0	2	2466
185	81	1	14	100	3	0	0	0	0	2	2495
186	82	1	23	94	3	1	0	0	0	0	2495
187	83	1	17	142	2	0	0	1	0	0	2495
188	84	1	21	130	1	1	0	1	0	3	2495

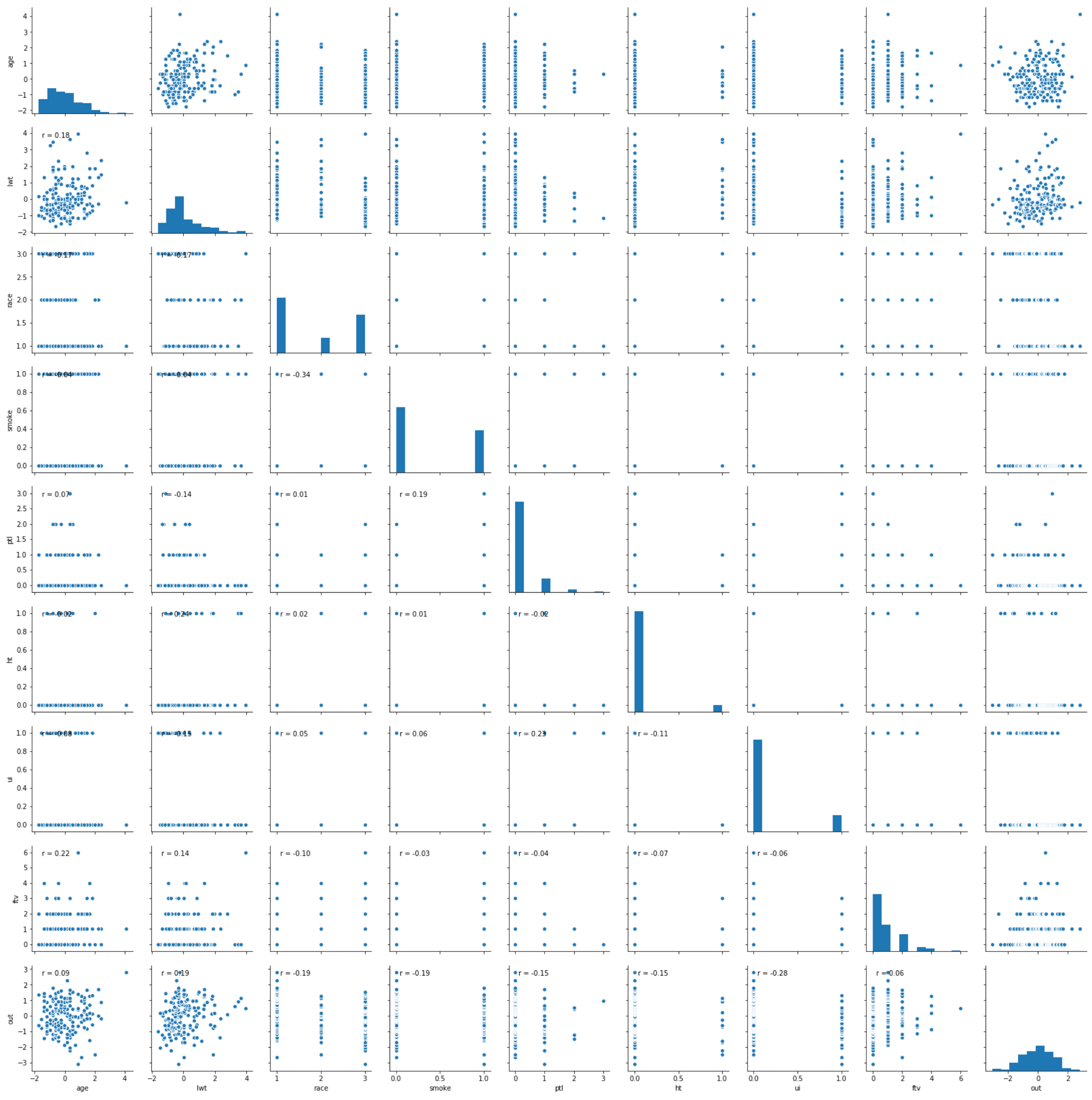
189 rows × 11 columns

In [30]:

```
g = sns.pairplot(pd.DataFrame(np.hstack((X, y[:, None])), columns=feat_names + [
'out']))
g.map_lower(corrfunc)
```

Out[30]:

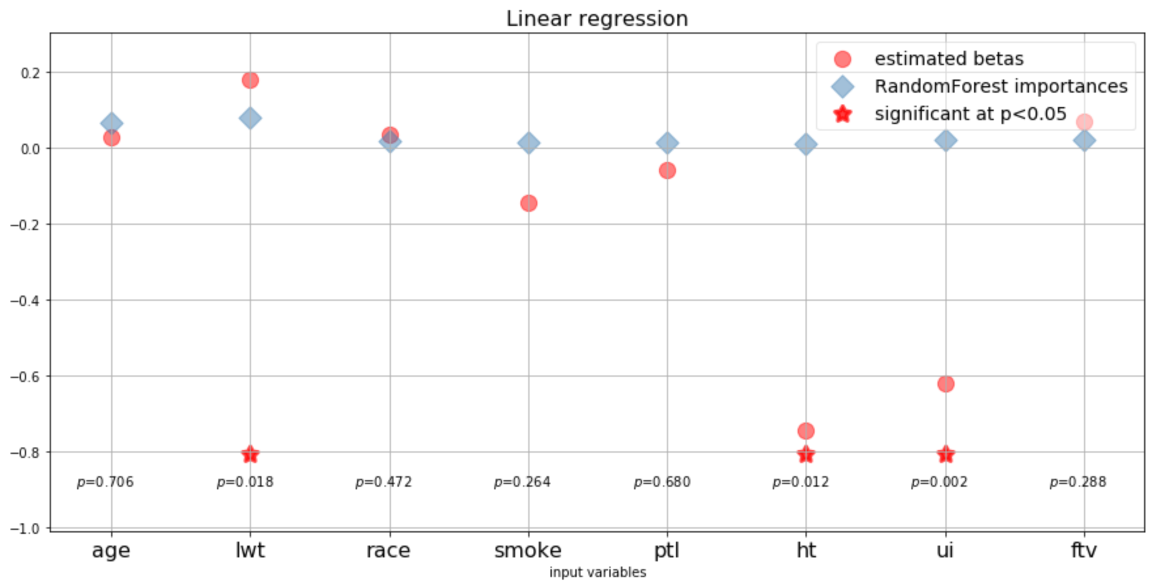
```
<seaborn.axisgrid.PairGrid at 0x12ea6bf28>
```

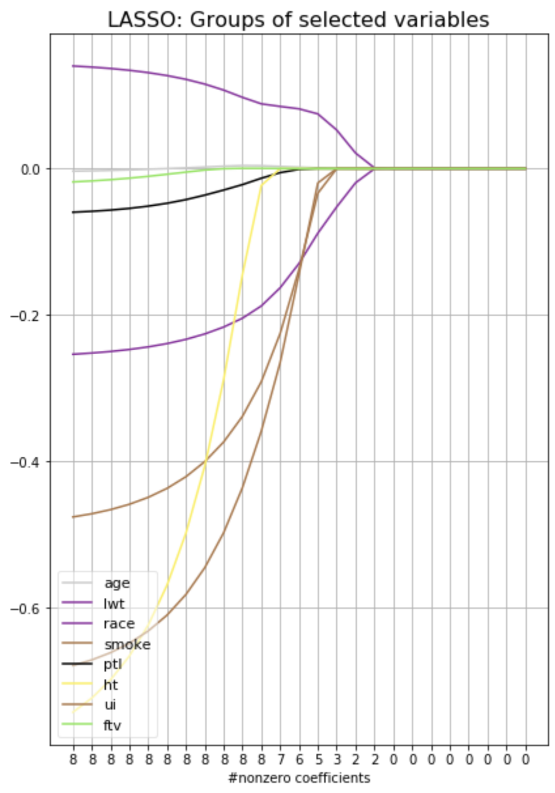


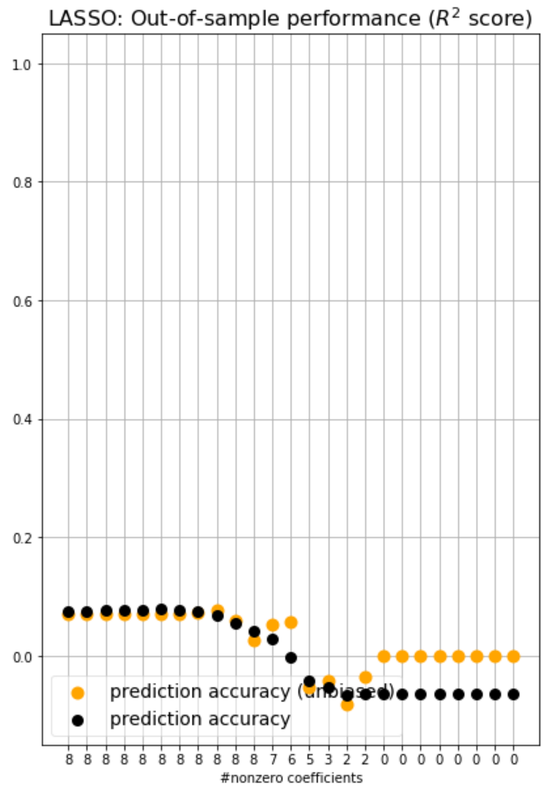
In [31]:

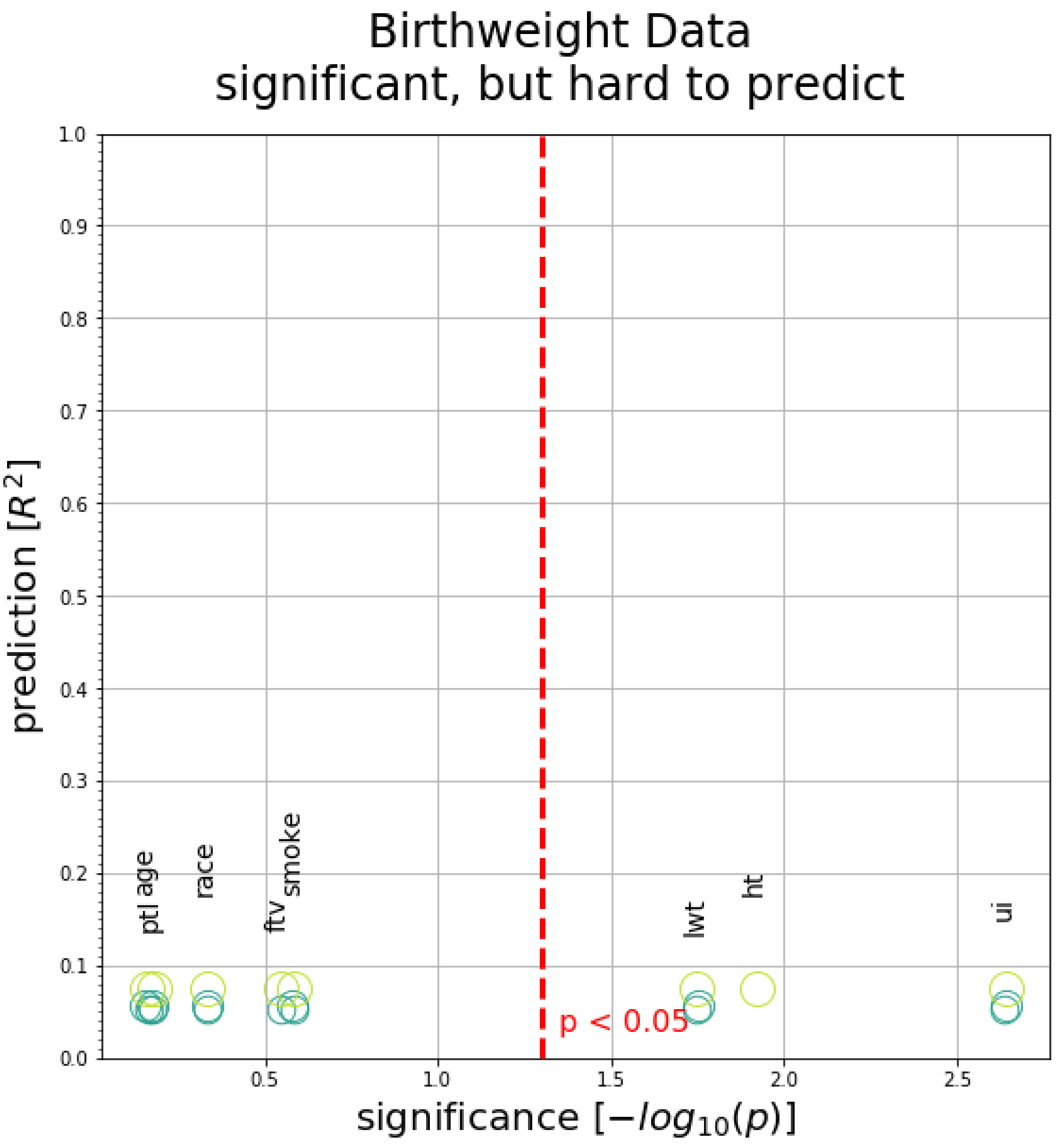
```
# ordinary least squares
model = OLS(y, X)
res = model.fit()
lr_coefs = res.params
lr_pvalues = res.pvalues

snr = (norm(a=lr_coefs, ord=2) ** 2) / (norm(a=res.resid, ord=2) ** 2)
print('Signal-to-noise ratio: %.4f' % snr)

rf_cmp.fit(X, y)
rf_cmp.feature_importances_

# compute Lasso regularization paths
C_grid = np.logspace(-2.5, 0.25, 25)
coef_list, acc_list, nonzero_list, unbiased_acc_list = compute_Lasso_regpath(X,
y, C_grid)

plot_lr(None, lr_coefs, lr_pvalues, feat_names, rf_cmp_coef=rf_cmp.feature_impor
tances_ * np.mean(np.abs(lr_coefs)))
path_colors = plot_regr_paths(coef_list, acc_list, nonzero_list, C_grid, feat_na
mes, unbiased_acc_list)


fig = infpred_plot(unbiased_acc_list, lr_pvalues, coef_list, feat_names)
fig.suptitle('Birthweight Data\nsignificant, but hard to predict',
             fontsize=24, fontweight=150)
fig.savefig('reg-case4.pdf', bbox_inches='tight')
```

```
Signal-to-noise ratio: 0.0062
alpha: 0.0032 acc: 0.07 / 0.07 (unbiased) active_coefs: 8
alpha: 0.0041 acc: 0.07 / 0.07 (unbiased) active_coefs: 8
alpha: 0.0054 acc: 0.08 / 0.07 (unbiased) active_coefs: 8
alpha: 0.0070 acc: 0.08 / 0.07 (unbiased) active_coefs: 8
alpha: 0.0091 acc: 0.08 / 0.07 (unbiased) active_coefs: 8
alpha: 0.0118 acc: 0.08 / 0.07 (unbiased) active_coefs: 8
alpha: 0.0154 acc: 0.08 / 0.07 (unbiased) active_coefs: 8
alpha: 0.0200 acc: 0.08 / 0.07 (unbiased) active_coefs: 8
alpha: 0.0261 acc: 0.07 / 0.08 (unbiased) active_coefs: 8
alpha: 0.0340 acc: 0.05 / 0.06 (unbiased) active_coefs: 8
alpha: 0.0442 acc: 0.04 / 0.03 (unbiased) active_coefs: 8
alpha: 0.0576 acc: 0.03 / 0.05 (unbiased) active_coefs: 7
alpha: 0.0750 acc: -0.00 / 0.06 (unbiased) active_coefs: 6
alpha: 0.0976 acc: -0.04 / -0.05 (unbiased) active_coefs: 5
alpha: 0.1271 acc: -0.05 / -0.04 (unbiased) active_coefs: 3
alpha: 0.1655 acc: -0.07 / -0.08 (unbiased) active_coefs: 2
alpha: 0.2154 acc: -0.06 / -0.04 (unbiased) active_coefs: 2
alpha: 0.2805 acc: -0.06 / 0.00 (unbiased) active_coefs: 0
alpha: 0.3652 acc: -0.06 / 0.00 (unbiased) active_coefs: 0
alpha: 0.4754 acc: -0.06 / 0.00 (unbiased) active_coefs: 0
alpha: 0.6190 acc: -0.06 / 0.00 (unbiased) active_coefs: 0
alpha: 0.8058 acc: -0.06 / 0.00 (unbiased) active_coefs: 0
alpha: 1.0491 acc: -0.06 / 0.00 (unbiased) active_coefs: 0
alpha: 1.3659 acc: -0.06 / 0.00 (unbiased) active_coefs: 0
alpha: 1.7783 acc: -0.06 / 0.00 (unbiased) active_coefs: 0
2.63386052717
1.91596042715
1.74389488205
0.578152099724
0.540222476357
0.326220298512
0.167438270664
0.151079649374
skipping 1
skipping 2
skipping 3
skipping 4
skipping 5
skipping 6
skipping 7
skipping 8
skipping 9
skipping 12
skipping 14
skipping 15
skipping 16
skipping 17
skipping 18
skipping 19
skipping 20
skipping 24
```


Linear regression
estimated betas
RandomForest importances
significant at p<0.05
p=0.706
p=0.018
p=0.472
p=0.264
p=0.680
p=0.012
p=0.002
p=0.288
age
lwt
race
smoke
ptl
ht
ui
ftv
input variables


LASSO: Groups of selected variables
age
lwt
race
smoke
ptl
ht
ui
ftv
#nonzero coefficients


LASSO: Out-of-sample performance (R^2 score)
prediction accuracy (unbiased)
prediction accuracy
#nonzero coefficients



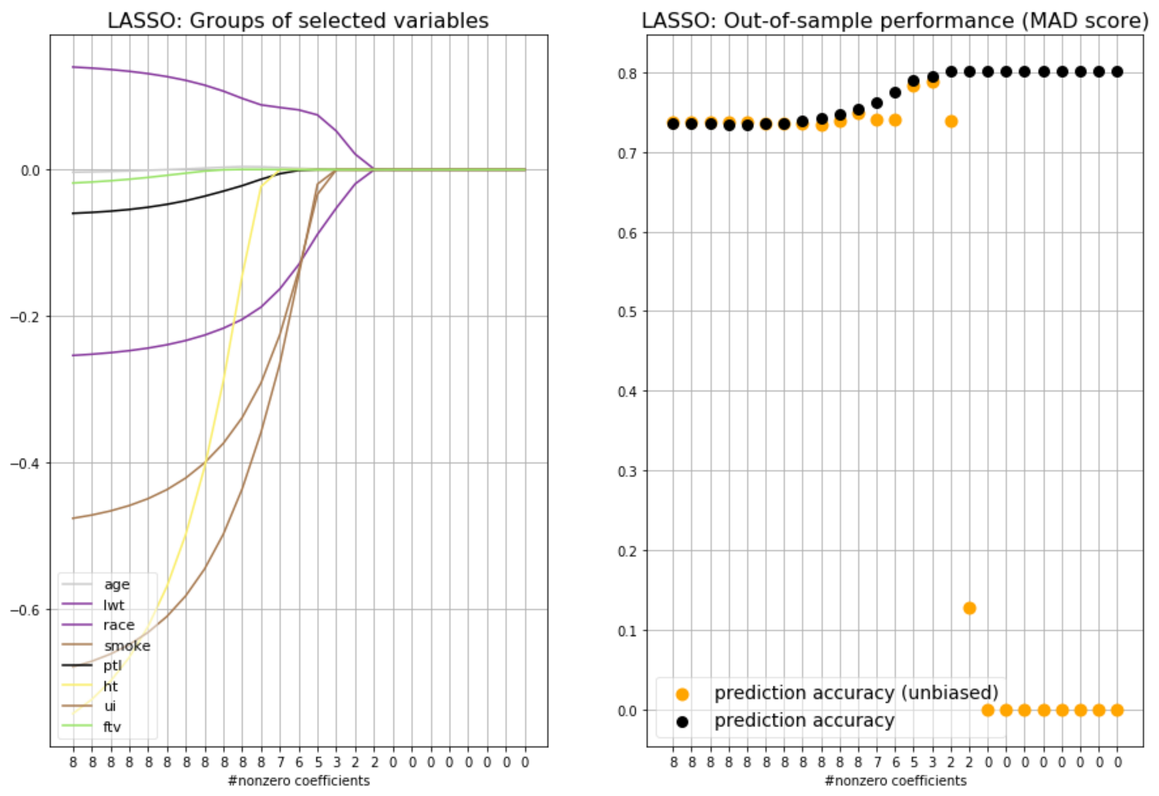
Birthweight Data
significant, but hard to predict
prediction [R^2]
significance [$-log_{10}(p)$]
p < 0.05
ptl
age
race
ftv
smoke
lwt
ht
ui
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.5
1.0
1.5
2.0
2.5

In [32]:

```
C_grid = np.logspace(-2.5, 0.25, 25)
coef_list, acc_list, nonzero_list, unbiased_acc_list = compute_Lasso_regpath(X,
y, C_grid, metric=mean_absolute_error, verbose=False)
plot_regr_paths(coef_list, acc_list, nonzero_list, C_grid, feat_names, unbiased_
acc_list, metric=mean_absolute_error)
```

Out[32]:

```
array(['#CCCCCC', '#85359C', '#85359C', '#A7794F', '#000000', '#FBEF
69',
       '#A7794F', '#98E466'],
      dtype='<U7')
```



In [33]:

```
sel_w_pvals = fwd_stepwise_selection(pd.DataFrame(X, columns=feat_names), y, ver
bose=True)
print('Forward-stepwise selection: ' + ' -> '.join(sel_w_pvals))
```

```
Add  ui                              with p-value 7.51844e-05
Add  race                            with p-value 0.0099902
Add  smoke                           with p-value 0.000239631
Add  ht                              with p-value 0.01275
Add  lwt                             with p-value 0.038581
Add  ptl                             with p-value 0.614145
Add  ftv                             with p-value 0.732379
Add  age                             with p-value 0.977929
Forward-stepwise selection: ui -> race -> smoke -> ht -> lwt -> ptl
-> ftv -> age
```

conclusion:

- significant, but challenging to predict (10% population variance)
- not explained by sample size that is relatively low (n=189)
- 3/8 input variables significant, but 7/8 necessary for low R=0.1 accuracy
- in CS, also the in-sample R^2 score is bad (!): 0.141
- It is an example that significance offers only weak insight on predictability -> we are missing additional information

In [34]:

```
res.summary(xname=feat_names)
```

Out[34]:

OLS Regression Results

Dep. Variable:	y	**R-squared:**	0.141
Model:	OLS	**Adj. R-squared:**	0.103
Method:	Least Squares	**F-statistic:**	3.724
Date:	Sun, 20 May 2018	**Prob (F-statistic):**	0.000468
Time:	17:30:11	**Log-Likelihood:**	-253.78
No. Observations:	189	**AIC:**	523.6
Df Residuals:	181	**BIC:**	549.5
Df Model:	8		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
age	0.0275	0.073	0.378	0.706	-0.116	0.171
lwt	0.1773	0.074	2.387	0.018	0.031	0.324
race	0.0322	0.045	0.721	0.472	-0.056	0.120
smoke	-0.1462	0.130	-1.120	0.264	-0.404	0.111
ptl	-0.0613	0.148	-0.413	0.680	-0.354	0.232
ht	-0.7446	0.294	-2.534	0.012	-1.325	-0.165
ui	-0.6217	0.201	-3.089	0.002	-1.019	-0.225
ftv	0.0683	0.064	1.065	0.288	-0.058	0.195

Omnibus:	0.618	**Durbin-Watson:**	0.417
Prob(Omnibus):	0.734	**Jarque-Bera (JB):**	0.748
Skew:	-0.080	**Prob(JB):**	0.688
Kurtosis:	2.737	**Cond. No.**	9.62

Additional Excericse: Primary biliary cirrhosis

In [35]:

```
import pandas as pd
df_cir = pd.read_excel('sources_medical_datasets/_Mayo_Clinic_primary_biliary_ci
rrhosis_pbc.xls')
```

```
*** No CODEPAGE record, no encoding_override: will use 'ascii'
```

In [36]:

```
df_cir
```

Out[36]:

	bili	albumin	stage	protime	sex	fu.days	age	spiders	hepatom
0	14.500000	2.60	4.0	12.2	female	400	58.765228	present	present
1	1.100000	4.14	3.0	10.6	female	4500	56.446270	present	present
2	1.400000	3.48	4.0	12.0	male	1012	70.072556	absent	absent
3	1.800000	2.54	4.0	10.3	female	1925	54.740589	present	present
4	3.400000	3.53	3.0	10.9	female	1504	38.105408	present	present
5	0.800000	3.98	3.0	11.0	female	2503	66.258728	absent	present
6	1.000000	4.09	3.0	9.7	female	1832	55.534565	absent	present
7	0.300000	4.00	3.0	11.0	female	2466	53.056812	absent	absent
8	3.200000	3.08	2.0	11.0	female	2400	42.507870	present	absent
9	12.600000	2.74	4.0	11.5	female	51	70.559891	present	absent
10	1.400000	4.16	4.0	12.0	female	3762	53.713894	present	present
11	3.600000	3.52	4.0	13.6	female	304	59.137577	present	absent
12	0.700000	3.85	3.0	10.6	female	3577	45.689255	absent	absent
13	0.800000	2.27	4.0	11.0	male	1217	56.221767	absent	present
14	0.800000	3.87	3.0	11.0	female	3584	64.646133	absent	absent

	bili	albumin	stage	protime	sex	fu.days	age	spiders	hepatom
15	0.700000	3.66	3.0	10.8	female	3672	40.443531	absent	absent
16	2.700000	3.15	4.0	10.5	female	769	52.183437	absent	present
17	11.400000	2.80	4.0	12.4	female	131	53.930183	present	present
18	0.700000	3.56	3.0	11.0	female	4232	49.560574	absent	present
19	5.100000	3.51	4.0	13.0	female	1356	59.953457	absent	present
20	0.600000	3.83	4.0	11.4	male	3445	64.188911	present	present
21	3.400000	3.63	4.0	11.6	female	673	56.276524	present	absent
22	17.400000	2.94	4.0	11.7	female	264	55.967144	present	present
23	2.100000	4.00	2.0	9.9	male	4079	44.520191	absent	present
24	0.700000	4.10	2.0	11.3	female	4127	45.073238	absent	absent
25	5.200000	3.68	3.0	9.9	female	1444	52.024639	present	present
26	21.600000	3.31	4.0	12.0	female	77	54.439426	present	present
27	17.200001	3.23	4.0	13.0	female	549	44.947296	present	present
28	0.700000	3.78	2.0	10.6	female	4509	63.876797	absent	absent
29	3.600000	2.54	4.0	11.0	female	321	41.385353	present	present
...	...	...	...	...	...	...	...	...	...
388	0.700000	3.06	4.0	10.0	female	1581	67.000000	NaN	NaN

	bili	albumin	stage	protime	sex	fu.days	age	spiders	hepatom
389	3.000000	3.15	3.0	10.0	male	1419	68.000000	NaN	NaN
390	1.200000	2.80	2.0	11.0	female	1443	41.000000	NaN	NaN
391	0.400000	3.03	3.0	10.9	female	1368	69.000000	NaN	NaN
392	0.700000	2.96	4.0	9.9	female	193	52.000000	NaN	NaN
393	2.000000	3.07	4.0	12.1	female	1367	57.000000	NaN	NaN
394	1.400000	3.98	1.0	11.0	female	1329	36.000000	NaN	NaN
395	1.600000	3.48	2.0	10.2	female	1343	50.000000	NaN	NaN
396	0.500000	3.65	4.0	10.2	female	1328	64.000000	NaN	NaN
397	7.300000	3.49	4.0	10.9	female	1375	62.000000	NaN	NaN
398	8.100000	2.82	2.0	10.4	female	1260	42.000000	NaN	NaN
399	0.500000	3.34	2.0	10.6	female	1223	44.000000	NaN	NaN
400	4.200000	3.19	4.0	11.1	female	935	69.000000	NaN	NaN
401	0.800000	3.01	3.0	10.6	female	943	52.000000	NaN	NaN
402	2.500000	3.33	4.0	10.8	female	1141	66.000000	NaN	NaN
403	4.600000	3.60	3.0	10.4	female	1092	40.000000	NaN	NaN
404	1.000000	3.64	3.0	10.6	female	1150	52.000000	NaN	NaN
405	4.500000	2.68	4.0	11.5	female	703	46.000000	NaN	NaN
406	1.100000	3.69	3.0	10.8	male	1129	54.000000	NaN	NaN

	bili	albumin	stage	protime	sex	fu.days	age	spiders	hepatom
407	1.900000	3.17	3.0	10.7	female	1086	51.000000	NaN	NaN
408	0.700000	3.73	3.0	10.8	female	1067	43.000000	NaN	NaN
409	1.500000	3.81	3.0	10.8	female	1072	39.000000	NaN	NaN
410	0.600000	3.57	3.0	10.6	female	1119	51.000000	NaN	NaN
411	1.000000	3.58	3.0	10.8	female	1097	67.000000	NaN	NaN
412	0.700000	3.23	3.0	10.8	female	989	35.000000	NaN	NaN
413	1.200000	2.96	3.0	10.9	female	681	67.000000	NaN	NaN
414	0.900000	3.83	4.0	11.2	female	1103	39.000000	NaN	NaN
415	1.600000	3.42	3.0	9.9	female	1055	57.000000	NaN	NaN
416	0.800000	3.75	3.0	10.4	female	691	58.000000	NaN	NaN
417	0.700000	3.29	4.0	10.6	female	976	53.000000	NaN	NaN

418 rows × 19 columns