In [1]:

```
from IPython import display
def hide_code_in_slideshow():
    import os
    uid = os.urandom(8).encode("hex")
    html = """<div id="%s"></div>
    <script type="text/javascript">
        $(function(){
            var p = $("#%s");
            if (p.length==0) return;

            while (!p.hasClass("cell")) {
                p=p.parent();

                if (p.prop("tagName") =="body") return;
            }
            var cell = p;
            cell.find(".input").addClass("hide-in-slideshow")
        });
    </script>""" % (uid, uid)
    display.display_html(html, raw=True)
```

Feature Importance outline

Feature importance

- Introduction and motivation for discussing feature importance:
  - Define feature importance (using a fuzzy definition -- rank features by how much they "*contribute*" to the prediction function).
  - Feature importance measures are frequently reported, in part because many packages make them easy to compute/visualize.
    - Show google image search results
  - They can be potentially misleading. Important to understand potential pitfalls.
  - Utility of feature importance:
    - Feature selection -- use votes example from original Breiman Random Forests paper.
    - Sanity checking models/detecting leakage (TODO: see if I can find an example where feature importance show some feature unexpectedly popping since due to leakage).
- Framing feature importance methods:
  - Divide into two classes:
    - Methods that exploit the structure of the prediction function or learning algorithm (call these function-specific).
    - Methods that are agnostic (i.e. can be applied to any black box prediction function).
- Function-specific methods:
  - Mean decrease impurity:
    - Frame running example:
      - Introduce the iris dataset and classification problem.
      - graphviz some shallow tree on the iris dataset (see below).
      - **Ask students** which features seem "important" as a turn and talk. Have some subset share answers without explanation.
    - Introduce MDE:

$$Imp(X_m) = \frac{1}{N_T} \sum_{T} \sum_{t \in T : v(s_t) = X_m} p(t) \Delta i(s_t, t)$$

    - Show from scratch implimentation (see lab_outline_and_mean_decrease_impurity.ipynb).
    - Show correspondance with sklearn's implementation.
    - **Ask students** what other classifiers we could extend this too (Random Forests/GBMs) and how (averaging).
    - Show RF importance for the iris problem.
    - Say there are variants:
      - Example: CART implementation exposes a knob to add weight for use of a feature as a surrogate split.
  - Absolute coefficients in a linear model:
    - **Ask students** how we could determine feature importance in a linear model.
    - Show some example (TODO) of extracting absolute βs from a model.
    - **Ask students**: How would this interact with preprocessing?
- Model agnostic methods:
  - Frame the general problem for global feature importance:

        - Another framing of feature importance -- we are trying to identify how much each feature independently contributes to risk reduction in the learned model.
        - **Ask students**: How could we do this for an arbitrary black box prediction function?
        - **Hint (fragment slide)**: Imagine you were tasked with constructing a synthetic dataset with an *unimportant* feature -- how could you construct it? Given this insight, what operation could be applied to a feature that would be expected to have (a) no impact on empirical risk for unimportant features, and (b) decrease performance for important featuers?
    - Permutation importance:
        - Give Breimans original OOB permutation feature importance.
        - Say that the OOB version exploits bootstrapping in RFs, but can just use a validation set.
        - Show example (using ELI5 implementation) over the iris problem.
        - **Ask students**: This method permute features to get a measure of feature importance. Let's extend this concept a bit -- how could permuting the target be useful in interogating the performance of a model?
        - http://jmlr.csail.mit.edu/papers/volume11/ojala10a/ojala10a.pdf (http://jmlr.csail.mit.edu/papers/volume11/ojala10a/ojala10a.pdf)
        - For fun show this using permutation_test_score for the iris data.
- Pitfalls:
    - Correlated features
        - Show the GBM feature importance for duplicated or highly correlated features (TODO: think about which is better for this purpose) (from lab_outline_and_mean_decrease_impurity.ipynb).
        - **Ask students**: Interpret this plot. What can we say about the features/model?
        - Show same plot for enet, and ask same question -- hopefully students will recall that (at least in the context of linear models) our conversations about feature correlation.
        - Show the elastnic net bound result as review, and primer to think about correlation issues.
        - Show correlation matrix/matrices (duplicated and/or highly correlated), and known data generating process.
        - **Ask students**: Given what we know about (i) linear methods, and (ii) trees, what does this show us about potential pitfalls in interpreting feature importance plots?
        - **Ask students**: How would this impact SelectFromModel feature selection procedures (ala sklearn) which select the most important features from a model based on either absolute coefficients or feature importance scores? Why might we want to use RFE?

PDPs

- Motivation and introduction to partial dependence plots
    - Imagine we have a subset of features we think are important.
        - This could be based on "feature importance" scores or coefficients, or other reasons (i.e. prior knowledge/research questions/etc.).
    - We may want to dig deeper to explain the relationship between our predictions and these features.
        - **Ask students**: Why? If we have MDI feature importance scores in hand, what do we not know?
            - Directionality:
                - Note in reality we probably have complex, non-monotonic relationships
                - However even if we have a monotonic relationship, or even linear, our MDI wouldn't give any indication on the direction -- obviously weights in a linear model would.

    - Partial dependence plots let us dig deeper and visualize the dependence of our prediction function (i.e. predict/predict_proba) on one or two of these features. Can't easily go higher-dimensional (Why not? Can't visualize).
    - Show basic math (marginal and empirical estimate -- see https://arxiv.org/pdf/1309.6392.pdf (https://arxiv.org/pdf/1309.6392.pdf) for useful framing).
- PDP examples:
    - Show sklearn example (see partial_dependence.ipynb).
    - **Ask students**: What does this plot show? How do we interpret it?
- PDP pitfalls:
    - Show the flat partial dependence plot from (https://arxiv.org/pdf/1309.6392.pdf (https://arxiv.org/pdf/1309.6392.pdf)) reproduced in partial_dependence.ipynb.
    - **Ask students**: What does this plot show?
    - Follow up with big reveal:
        - Show data generating process and X plot.
    - **Ask students**: What does this teach us? When might PDPs fail?
    - Share "not too strong" quote from Friedman's original work (see partial_dependence.ipynb).

Additional material

- If 100 minutes allows (what is your opinion, David?), the next steps would be:
    - Generate the ICE plot for the X data (figure 2 in https://arxiv.org/pdf/1309.6392.pdf (https://arxiv.org/pdf/1309.6392.pdf))
    - Take this as a launching point for point out that our progression has been from:
        - Global measures (feature importance) that don't necessarily describe structure (even directionality) of a relationship between a feature and target.
        - Marginalized measures showing average relationship between one or two features and the target.
        - Data-instance specific feature importance plots showing the importance of a feature, for each data instance, fixing all other feature values.
    - We can follow this thread it's conclusion -- attempting to develop model explanations that show the relative contribution of each feature to predictions locally (i.e. in the neighborhood of a specific instance):
        - LIME paper (https://arxiv.org/abs/1602.04938 (https://arxiv.org/abs/1602.04938)) as one example.

Feature Importance

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NYU
May 1st, 2018

Learning objectives

Feature Importance

- (Informally) define feature importance, and explain why exploring and presenting feature importance can be both (i) useful, and (ii) potentially misleading.
- Define and describe several feature importance methods that exploit the structure of the learning algorithm or learned prediction function.
- Describe a prediction-function-agnostic method for generating feature importance scores.
- Describe the limitations of these feature importance measures and understand cases where they "fail".

Partial Dependence Plots

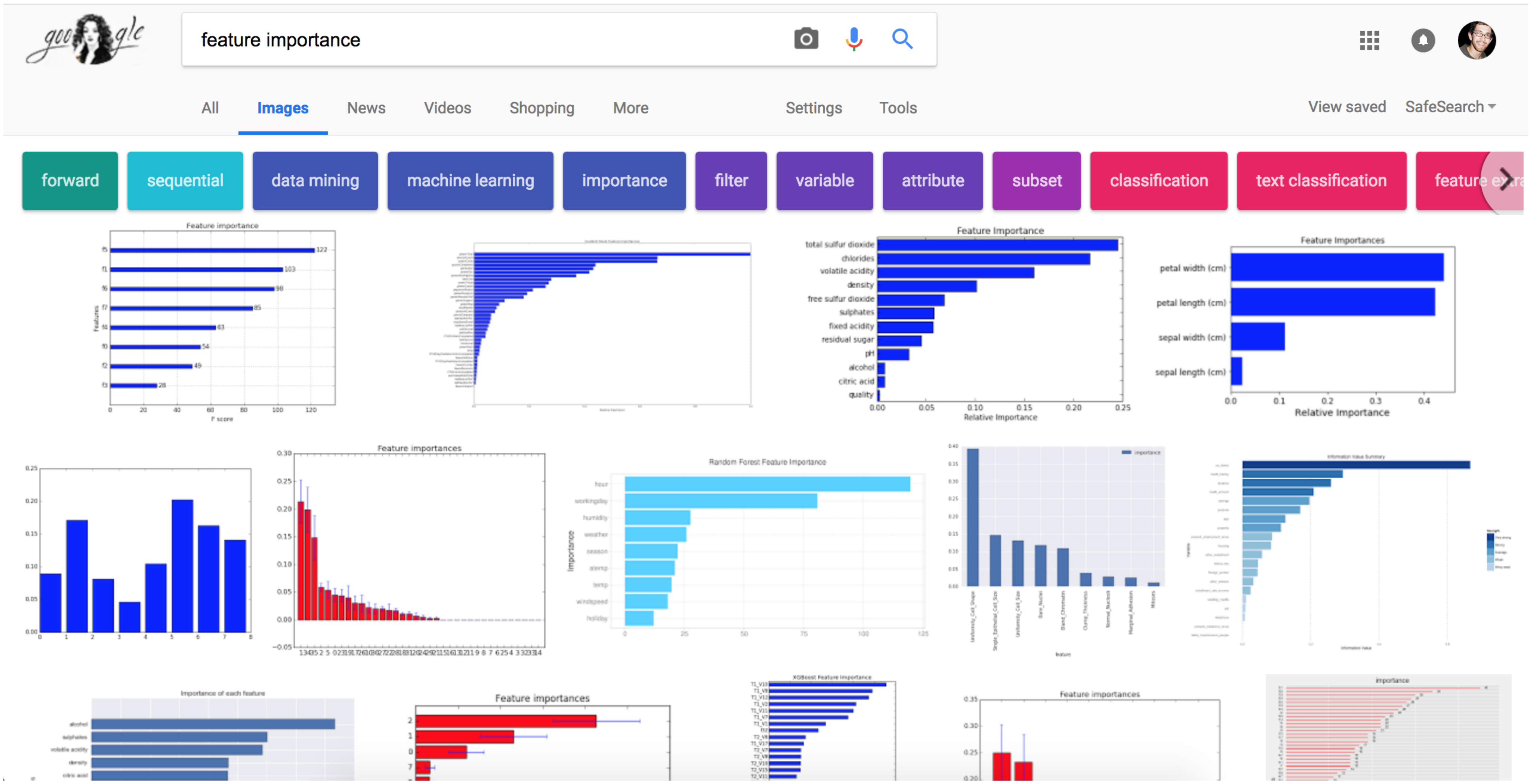
- Describe how partial dependence plots are generated.
- Describe the limitations of these plots, and some potential remedies.

Defining feature importance

- Problem setup -- we have some data $(x, y) \in (\mathbb{R}^d, \mathcal{Y})$, and a learned prediction function f.
- A feature importance method can be loosely understood as a function that maps each feature onto some score.
- These scores rank features by how much they "*contribute*" to the prediction function f.
  - Here "*contribute*" is defined separately for each method.
  - In general, *feature importance* is not consistently or rigorously defined.

Why we need to discuss feature importance

- It is easy to compute feature importance from many ML libraries.


feature importance
All
Images
News
Videos
Shopping
More
Settings
Tools
View saved
SafeSearch
forward
sequential
data mining
machine learning
importance
filter
variable
attribute
subset
classification
text classification
Feature importance
Feature Importance
Feature Importances
Relative Importance
Feature importances
Random Forest Feature Importance
Importance of each feature
XGBoost Feature Importance
importance

Why we need to discuss feature importance

- It is easy to compute feature importance from many ML libraries.
- This means feature importance bar charts show up all over, and it is important to understand:
    - How feature importance can be computed.
    - Potential pitfalls in over interpreting these scores.

Utility of feature importance scores

- **Question**: Why might feature importance scores be useful?

- Use for sanity checking a model -- do the features that are important seem reasonable, or do they suggest something strange is going on under the hood (i.e. leakage)?

- Share with clients/bosses to build trust and get buy-in on the prediction function.

- Use for feature selection -- can extract the top K features and retrain over this subset (ex: `sklearn.feature_selection.SelectFromModel`)

Feature selection example

- Breiman's original Random Forests paper showed feature importance for classification of political party based on 16 votes[1] (https://link.springer.com/content/pdf/10.1023/A:1010933404324.pdf):

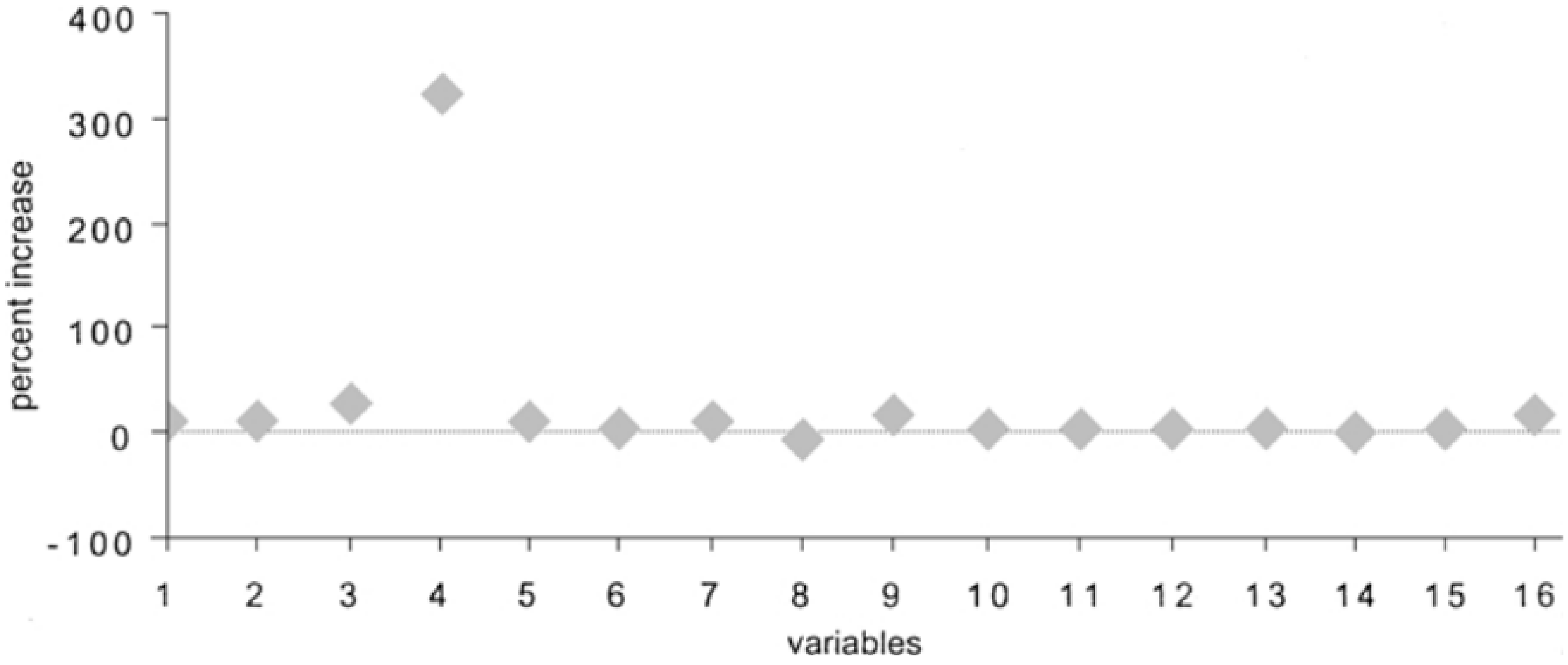


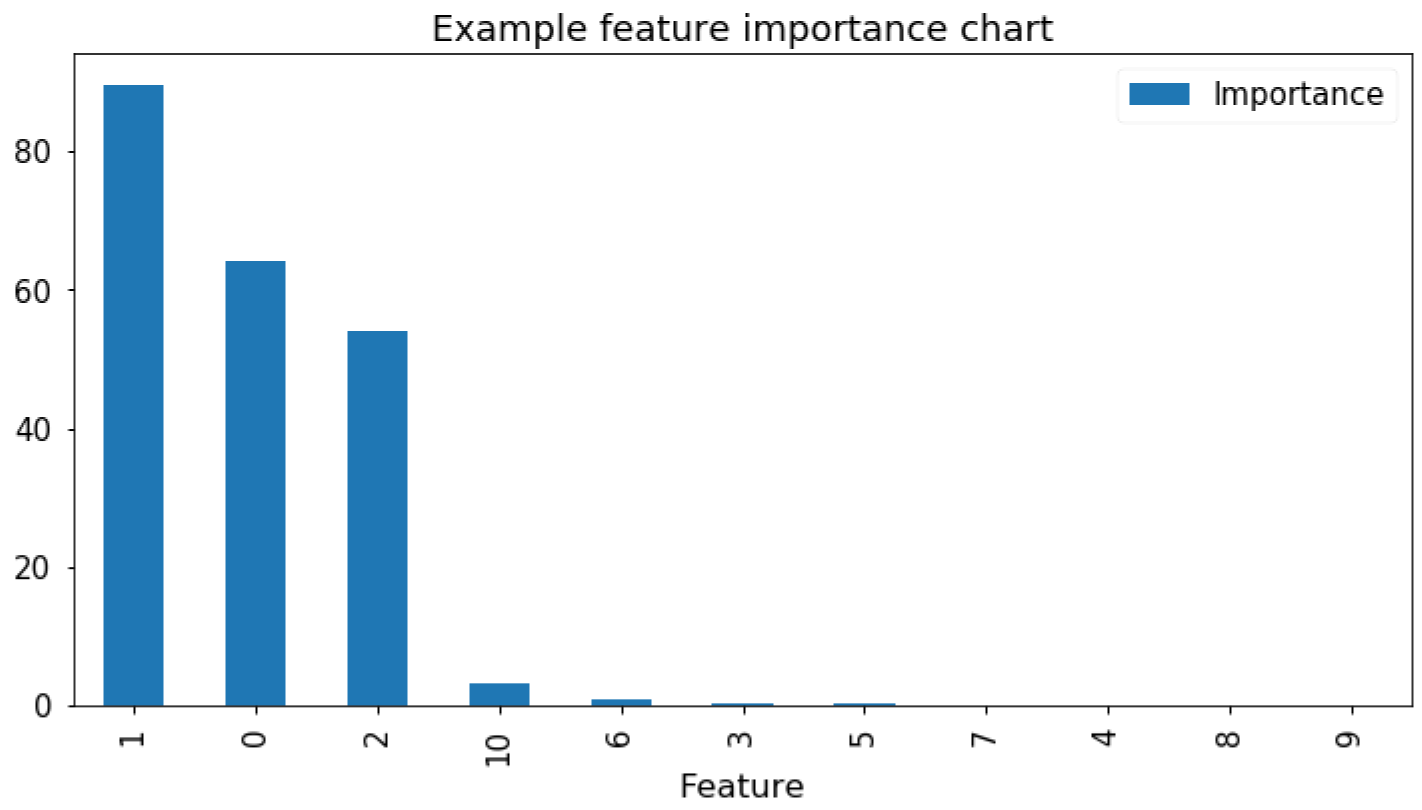
Figure 6. Measure of variable importance–votes data.

- *'We reran this data set using only variable 4. The test set error is 4.3%, about the same as if all variables were used.'*

First example/introducing the issues

- Consider the following feature importance plot for a regression problem with
$$\mathcal{Y} = \mathcal{A} = \mathbb{R}, X = \mathbb{R}^{11}$$

```
In [2]: hide_code_in_slideshow()
        from sklearn.datasets import make_regression
        from sklearn.model_selection import train_test_split
        from sklearn.linear_model import ElasticNetCV
        import pandas as pd
        import matplotlib.pyplot as plt
        import numpy as np
        import seaborn as sns
        sns.set_context('notebook', font_scale=1.5)
        %matplotlib inline

        X,y = make_regression(n_samples=1000, n_features=10,
                              n_informative=3,random_state=1234,
                              shuffle=False, noise=10)
        X = np.append(X, X[:,[0]], axis=1)
        train_X, test_X, train_y, test_y = train_test_split(X,y,
                                                             test_size=0.2,
                                                             random_state=1235)

        enet = ElasticNetCV(l1_ratio=np.array([.1, .5, .7, .9, .95, .99, 1]),
                            n_alphas=500,
                            normalize=True,
                            selection='random',
                            random_state=1351)
        enet.fit(train_X, train_y)

        coefs = pd.DataFrame({'Feature': np.arange(len(enet.coef_)),
                              'Importance': np.abs(enet.coef_)})
        coefs = coefs.set_index('Feature')\
                     .sort_values('Importance', ascending=False)

        fig, ax=plt.subplots(figsize=(12,6))
        plot = coefs.plot(kind='bar', title='Example feature importance chart', ax=ax)
```



- Question: What can we say about this prediction function, it features, and target?

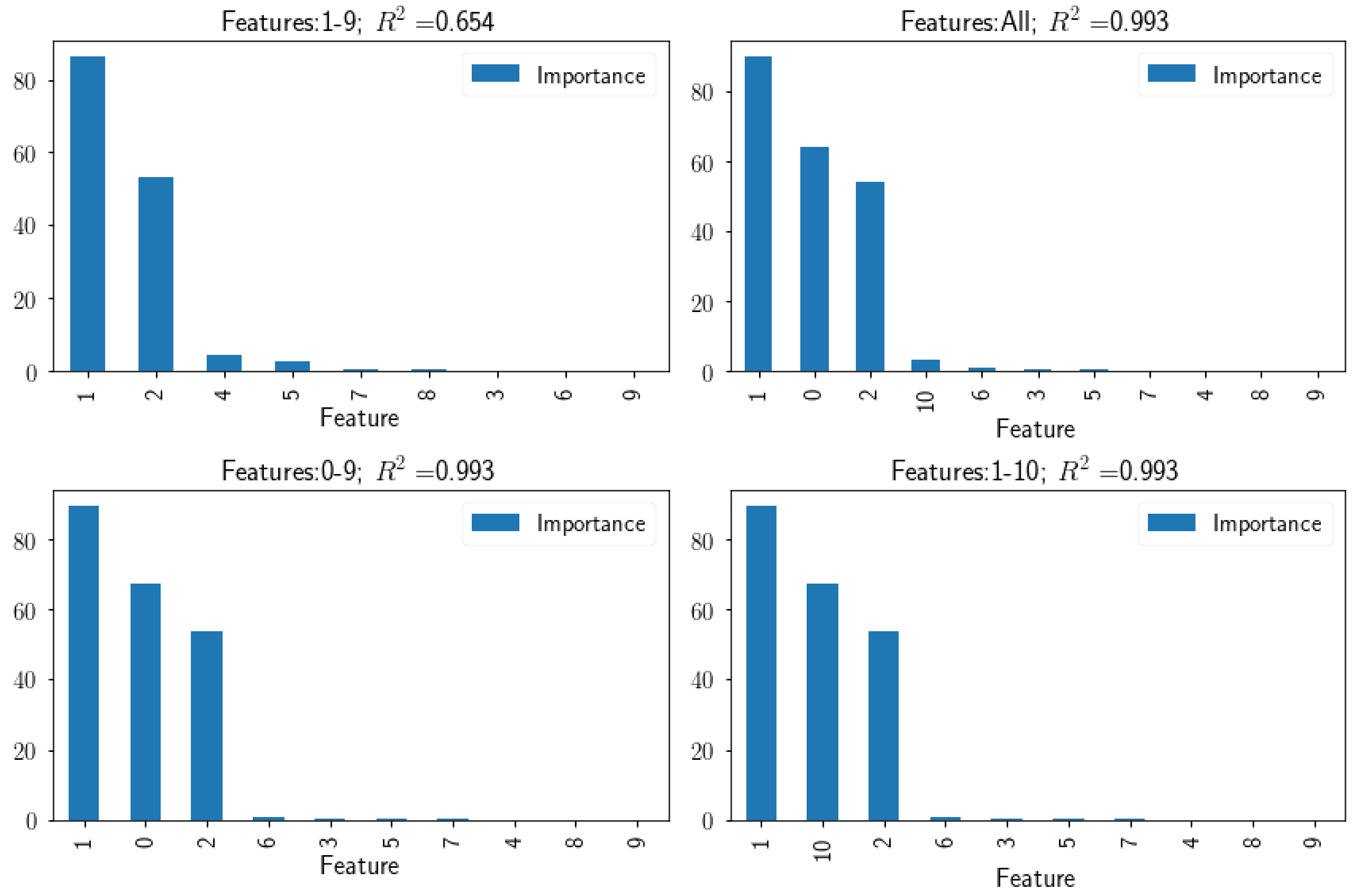
First example/introducing the issues (continued)

- Recall the full feature set includes features $\{0, \cdots, 10\}$.
- Let's compare both (a) test set performance (R^2), and (b) feature importance plots, for models trained on:
  - All features
  - Features $\{0, \cdots, 9\}$
  - Features $\{1, \cdots, 9\}$
  - Features $\{1, \cdots, 10\}$

First example/introducing the issues (continued)

- Recall the full feature set includes features $\{0, \cdots, 10\}$...

In [3]:
```
from matplotlib import rc
rc('text', usetex=True)

from sklearn.metrics import mean_squared_error
from math import floor

hide_code_in_slideshow()
features_to_test = {
    'All': np.arange(0,11),
    '0-9': np.arange(0,10),
    '1-9': np.arange(1,10),
    '1-10': np.arange(1,11)
}

fig, axarr = plt.subplots(ncols=2, nrows=2, figsize=(12,8))

i = 0
for model_name, features in features_to_test.items():
    col = i % 2
    row = int(floor(i/2))

    _train_X = train_X[:, features]
    _test_X = test_X[:, features]

    enet = ElasticNetCV(l1_ratio=np.array([.1, .5, .7, .9, .95, .99, 1]),
                        n_alphas=1000,
                        normalize=True,
                        selection='random',
                        random_state=1351)
    enet.fit(_train_X, train_y)

    coefs = pd.DataFrame({'Feature': features,
                          'Importance': np.abs(enet.coef_)})
    coefs = coefs.set_index('Feature')\
                 .sort_values('Importance', ascending=False)

    plot = coefs.plot(kind='bar', title='Typical feature importance chart', ax=axarr[(row,col)])

    title = 'Features:' + model_name + r'; $R^2$ =' + \
            str(round(enet.score(_test_X,test_y),3))

    axarr[(row,col)].set_title(title)

    i += 1
plt.tight_layout()
```



- What can we learn from this example?

First example/introducing the issues (continued)

- Here was the setup:

```
X,y = make_regression(n_samples=1000, n_features=10,
                      n_informative=3, random_state=1234,
                      shuffle=False, noise=10)
X = np.append(X, X[:,[0]], axis=1)
```

- Some things to keep in mind:
  - Interactions and correlated/dependent features makes intepretation tricky.
  - Feature importance $\neq$ dependence of target on feature
  - Feature importance $\approx$ contribution of feature to prediction function f
  - **This doesn't imply there do not exist other functions f' where features that are 'unimportant' in f are 'important'**

Where we're headed:

- With this in mind, we're going to look at a number of methods for measuring feature importance.
- We can devide these methods into two basic classes:
  - Algorithmic/prediction-function-specific methods: These exploit the structure of the learning algorithm/prediction function to construct some measure of the relative contribution of each feature.
  - Model agnostic methods: These don't make assumptions on the algorithm or structure of the prediction function; can be applied to any black-box predictor.

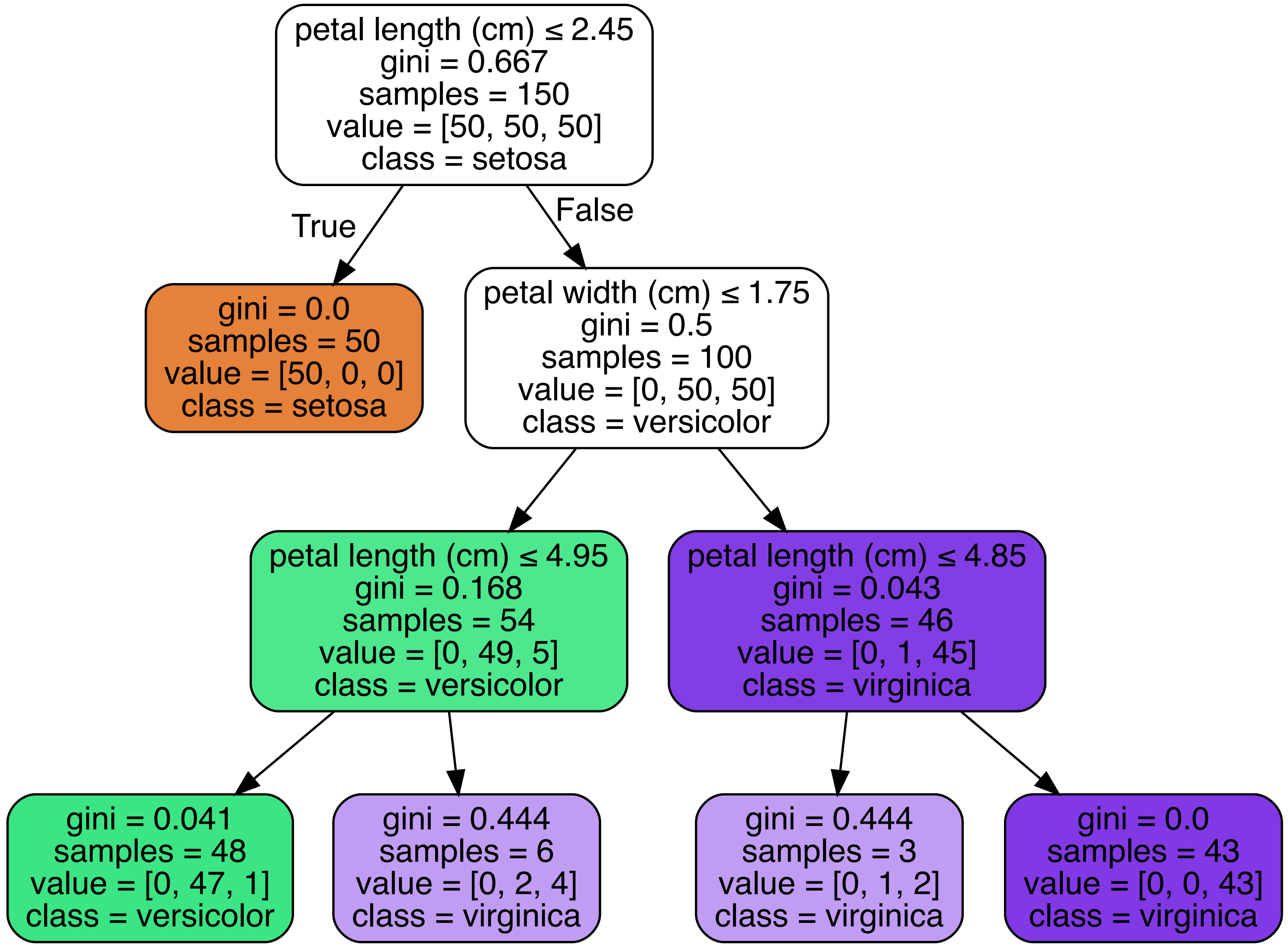
Prediction-function-specific: Trees

- Our first algorithm/prediction function specific methods will address decision trees.
- We'll use the Iris Dataset, which is a canonical classification dataset (first used by R.A. Fisher) with:
  - $\mathcal{Y} =$ {Setosa, Versicolour, Virginica} (three varieties of irises).
  - $X =$ [sepal length, sepal width, petal length, petal width] $\in \mathbb{R}^4$

Prediction-function-specific: Trees (Continued)

- Let's consider a shallow tree built on this data.

In [4]:
```python
hide_code_in_slideshow()
from sklearn.datasets import load_iris
from sklearn import tree
import graphviz

iris = load_iris()
clf = tree.DecisionTreeClassifier(max_depth=3)
clf = clf.fit(iris.data, iris.target)


dot_data = tree.export_graphviz(clf, out_file=None,
                                feature_names=iris.feature_names,
                                class_names=iris.target_names,
                                filled=True, rounded=True,
                                special_characters=True)
graph = graphviz.Source(dot_data)
display.display(graph)
```



- **Question**: Which of the feature ([sepal length, sepal width, petal length, petal width]) are most important? Why?

Prediction-function-specific: Trees (Continued)

Tree buiding reminders

- Consider node t in a decision tree built on N training data instances.
- Let node t have N_t node samples.
- We find the split s_t at node t such that t_L and t_R maximizes the decrease
$$\Delta i(s,t) = i(t) - p_L i(t_L) - p_R i(t_R)$$
where p_L and p_R are the probabilities an instance splits left and right, respectively, and $i(t)$ is some some impurity measure.

Prediction-function-specific: Trees (Continued)

Mean decrease impurity

- The **mean decrease impurity** $imp(X_m)$ for feature X_m is:
$$imp(X_m) = \sum_{v(s_t)=X_m} p(t)\Delta i(s_t,t)$$
Note $p(t) = N_t/N$ is the proportion of samples reaching node t and $v(s_t)$ is the variable used in split s_t.

Prediction-function-specific: Trees (Continued)

$$imp(X_m) = \sum_{v(s_t)=X_m} p(t)\Delta i(s_t,t)$$

- **Question**: When will a feature be considered more important under this metric?

- **Question**: Why is this an algorithm/prediction-function specific method?

Prediction-function-specific: Trees (Continued)

- Implementation:

In [8]:
```python
from collections import defaultdict
import numpy as np

def feature_importance_single_tree(tree, feature_names=iris.feature_names):
    # Returns normed feature importance for a single sklearn.tree
    # Note sklearn trees can handle instance weights, so we need
    # to use weighted_n_node_samples

    total_samples = np.sum(tree.weighted_n_node_samples)
    feature_importance = defaultdict(float)

    # Identify leaves as described in sklearn's plot_unveil_tree_structure.html
    is_leaf = (tree.children_right == tree.children_left)
    for ix in range(len(is_leaf)):
        if not is_leaf[ix]:
            impurity = tree.impurity[ix]
            split_feature = tree.feature[ix]
            num_at_node = tree.weighted_n_node_samples[ix]

            # Get left child contribution
            left_child = tree.children_left[ix]
            left_decrease = tree.weighted_n_node_samples[left_child]/num_at_node * \
                                tree.impurity[left_child]

            # Get right child contribution
            right_child = tree.children_right[ix]
            right_decrease = tree.weighted_n_node_samples[right_child]/num_at_node * \
                                tree.impurity[right_child]

            delta = impurity - left_decrease - right_decrease

            feature_importance[feature_names[split_feature]] \
                += num_at_node / total_samples * delta
    norm = np.sum(feature_importance.values())
    feature_importance = {key: val/norm for key, val in feature_importance.items()}
    return feature_importance
```

Prediction-function-specific: Trees (Continued)

- Implementation vs. sklearn

In [9]:
```
imp = feature_importance_single_tree(clf.tree_)
display.display(pd.Series(imp).rename('Importance').to_frame()\
                    .reset_index().rename(columns={'index':'Feature'}))
```

	Feature	Importance
0	petal length (cm)	0.585616
1	petal width (cm)	0.414384

In [10]:
```
display.display(pd.DataFrame({'Feature': iris.feature_names,
                                  'Importance':clf.feature_importances_})\
                    .sort_values('Importance', ascending=False))
```

	Feature	Importance
2	petal length (cm)	0.585616
3	petal width (cm)	0.414384
0	sepal length (cm)	0.000000
1	sepal width (cm)	0.000000

Prediction-function-specific: Trees (Continued)

- **Question**: How do we extend this to ensembles of trees?

- **Answer**: (Weighted) averages.
  - Ex: Random Forests with N_T trees:

$$Imp(X_m) = \frac{1}{N_T} \sum_T \sum_{t \in T : v(s_t) = X_m} p(t) \Delta i(s_t, t)$$

Prediction-function-specific: Trees (Continued)

- Implementation vs. sklearn

In [11]:
```python
from sklearn.ensemble import RandomForestClassifier
forest = RandomForestClassifier(n_estimators=100) # Not tuned - just example
forest.fit(iris.data, iris.target)
display.display(pd.DataFrame({'Feature': iris.feature_names,
                              'Importance':forest.feature_importances_})\
                 .sort_values('Importance', ascending=False))
```

	Feature	Importance
3	petal width (cm)	0.455781
2	petal length (cm)	0.415403
0	sepal length (cm)	0.102569
1	sepal width (cm)	0.026247

In [12]:
```python
forest_importance = defaultdict(float)
for tree in forest.estimators_:
    tree_importance = feature_importance_single_tree(tree.tree_)

    for key, val in tree_importance.items():
        forest_importance[key] += val
forest_importance = {key:val/len(forest.estimators_)\
                     for key, val in forest_importance.items()}

display.display(pd.Series(forest_importance).rename('Importance').to_frame()\
                 .reset_index().rename(columns={'index':'Feature'})\
                 .sort_values('Importance', ascending=False))
```

	Feature	Importance
1	petal width (cm)	0.455781
0	petal length (cm)	0.415403
2	sepal length (cm)	0.102569
3	sepal width (cm)	0.026247

Prediction-function-specific: Trees (Continued)

- Let's think about potential variants/extensions to mean decrease impurity.
- How could we handle surrogate splits?

- Commercial implementation of CART (https://www.salford-systems.com/support/faq/cart/what-is-variable-importance) adds contributions of surrogate splits:
  - $\Delta i(s_t, t)$ for primary split variable
  - $p^n \Delta i(s_t, t)$ for the n'th surrogate split variable (where $p \in [0, 1]$ is a user-selected hyperparameter).
- **Question**: Can we think of any other variants or extensions?

- Consider collapsing the importance of dummy-encoded categoricals.

Prediction-function-specific: Linear models

- **Question**: How can we measure feature importance in a linear model?

$$imp(X_m) = \left|w_m\right|$$

- **Question**: Per usual, how does this notion of importance interact with preprocessing?

Model-agnostic feature importance:

- We've discussed two methods for algorithm or prediction-function specific feature importance measures:
  - Trees (and their ensembles): Mean Decrease Impurity
  - Linear methods: Absolute weights
- **Question**: How could we determine the importance of input features for an arbitrary black box prediction function?

- Hint 1: Think about defining importance as by measuring how much each feature independently contributes to the performance of the learned model.

- Hint 2: Imagine you were tasked with constructing a synthetic dataset with an unimportant feature -- how could you construct it? Given this insight, what operation could be applied to a feature that would be expected to have (a) no impact on the test set score for unimportant features, and (b) decrease performance for important features?

Model-agnostic feature importance:

Permutation Importance

- Described by Breiman in the original Random Forests paper (using OOB sample).
- We describe it using an arbitrary held-out test set:

  1. Learn prediction function f on training data.
  2. Measure the performance of f on the test set - call this s_0.
  3. For each feature i in $[1, \cdots, D]$:
     A. Permute just this feature in the test set.
     B. Pass this permuted test set through f to obtain a new score s_i.
  4. Use either $s_0 - s_i$ (or some appropriate variant on this idea) as feature importance.

Model-agnostic feature importance:

Permutation Importance

- **Question**: Why bother permuting the feature? Why not just drop it entirely?

- **Question**: Why bother permuting the feature? Why not replace it with some noise, like $\mathcal{N}(0, 1)$?

Model-agnostic feature importance:

Permutation Importance

- **Question**: Is this any different than the following procedure? If so, how?

    1. Learn prediction function f on training data.
    2. Measure the performance of f on the test set - call this s_0.
    3. For each feature i in $[1, \cdots, D]$:
        A. Drop this feature from both the training and the test set.
        B. Learn a new prediction function without this feature -- call this function $f_{\setminus i}$
        C. Measure the performance of $f_{\setminus i}$ on the test set to obtain a new score s_i.
    4. Use either $s_0 - s_i$ as feature importance.

- **Key difference**: Permutation importance (plus $|w|$ and MDI) describe the importance of each feature to a particular prediction function f. We don't claim that a feature with low permutation importance in f couldn't have high importance in some other f'.

Feature importance pitfalls:

- To conclude our discussion of feature importance, we're going to look at an example to understand potential pitfalls.
- We will compare:
    - Permutation importance
    - MDI for a gradient boosting regressor
    - $|w|$ for an elastic net

Feature importance pitfalls: Problem set up

In [14]:

```
import numpy as np
size = 1000
x1 = np.random.uniform(-10,10,size)
z1 = np.random.uniform(-10,10,size)
x2 = z1 + np.random.normal(0,2,size)
x3 = z1 + np.random.normal(0,2,size)
x4 = z1 + np.random.normal(0,2,size)

def actual_function(x1,z1):
    return -1./2.*x1 + z1 + np.random.normal(0,1,len(x1))

y = actual_function(x1,z1)
X = np.stack([x1,x2,x3,x4]).T
```

- **Question**: Which feature is most important (i.e. contributes most to the true conditional mean function)?

- **Question**: Why might we expect this problem to challenge our feature importance methods?

In [43]:

```
hide_code_in_slideshow()
corr = pd.DataFrame(X).corr()
corr.index = ['$x_{}$'.format(x) for x in range(4)]
corr.columns = ['$x_{}$'.format(x) for x in range(4)]
display.display(display.Markdown('## Correlation matrix:'))
display.display(corr)
```

Correlation matrix:

	x_0	x_1	x_2	x_3
x_0	1.000000	-0.057013	-0.037270	-0.042008
x_1	-0.057013	1.000000	0.901286	0.898897
x_2	-0.037270	0.901286	1.000000	0.903997
x_3	-0.042008	0.898897	0.903997	1.000000

Feature importance pitfalls: Prediction functions

```
In [26]: from sklearn.model_selection import train_test_split
         from sklearn.ensemble import GradientBoostingRegressor
         from sklearn.model_selection import GridSearchCV

         train_X, test_X, train_y, test_y = train_test_split(X,y,test_size=0.2,
                                                             random_state=1345134)
         reg = GradientBoostingRegressor(n_estimators=200,subsample=0.5,
                                         random_state=3141)
         grid = GridSearchCV(reg,
                             param_grid={
                                 'max_leaf_nodes':[10,25,50],
                                 'min_samples_leaf':[10,25,50]
                             }, n_jobs=5, cv=5)
         grid = grid.fit(train_X, train_y)
```

```
In [27]: imp = pd.DataFrame({'Feature': ['$x_{}$'.format(i) for i in range(1,5)],
                             'GBM Importance':grid.best_estimator_.feature_importances_})
```

Feature Importance: Permutation Importance implementation

```
In [28]: import eli5
         from eli5.sklearn import PermutationImportance

         perm = PermutationImportance(grid)
         perm.fit(test_X, test_y)

         imp['GBM Permutation'] = perm.feature_importances_
```

Feature Importance: Elastic Net

In [29]:
```
from sklearn.linear_model import ElasticNetCV

enet = ElasticNetCV(l1_ratio=np.array([.1, .5, .7, .9, .95, .99, 1]),
                    n_alphas=500,
                    normalize=True,
                    selection='random',
                    cv=5,
                    random_state=1351)
enet.fit(train_X, train_y)

imp['Elastic Net $\\vert w \\vert$'] = np.abs(enet.coef_)

perm2 = PermutationImportance(enet)
perm2.fit(test_X, test_y)

imp['Elastic Net Permutation'] = perm2.feature_importances_
```

Feature Importance: Results

- Recall $E[y \mid x_1, z] = -\frac{1}{2}x_1 + z$ However, we don't observe z -- instead have 3 indepedent noisy observations x_2, x_3, x_4. Trying to estimate $E[y \mid x_1, \cdots, x_4]$

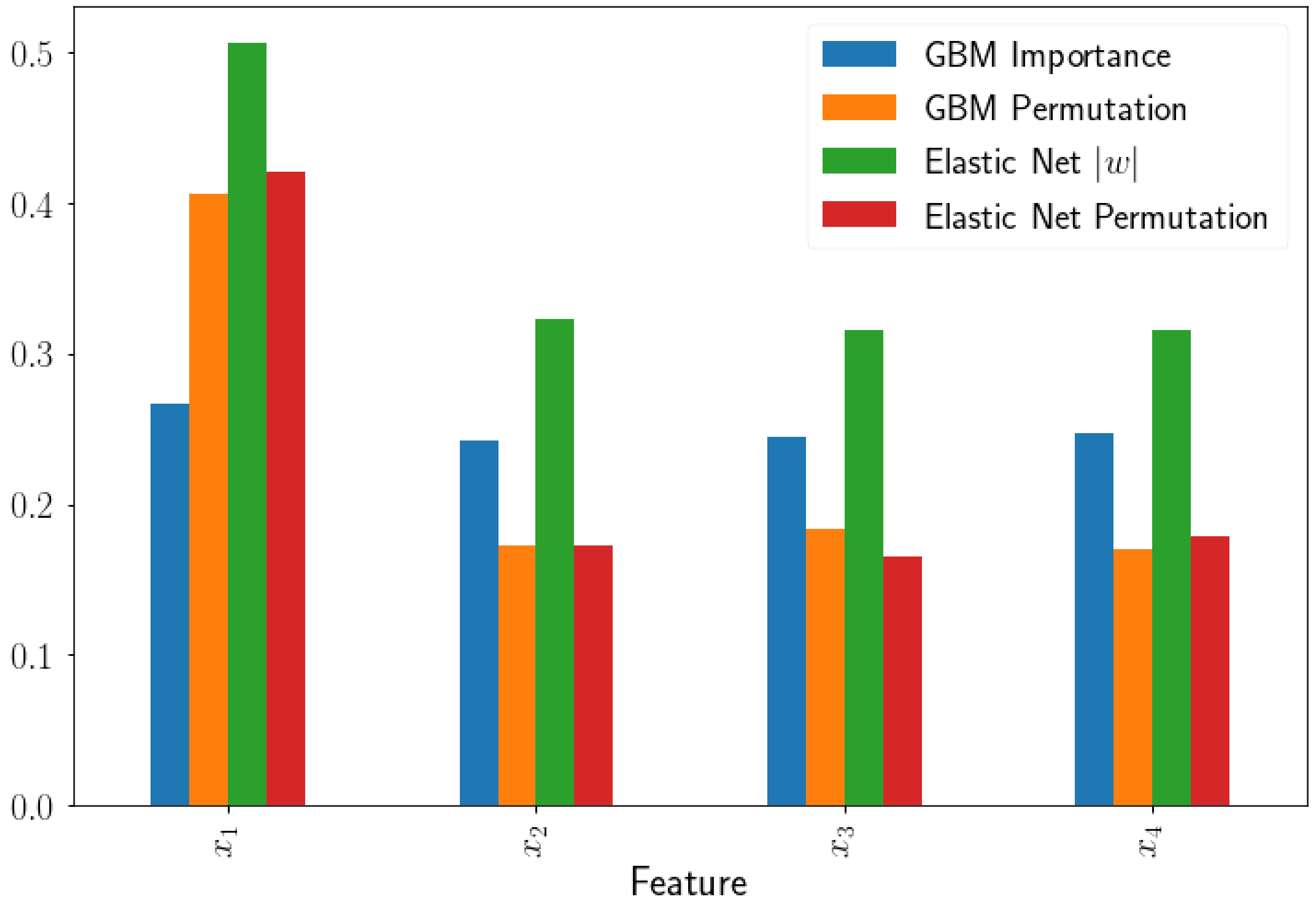
In [30]:
```
hide_code_in_slideshow()
display.display(imp.set_index('Feature'))
```

	GBM Importance	GBM Permutation	Elastic Net $\vert w \vert$	Elastic Net Permutation
Feature				
x_1	0.266826	0.406382	0.505771	0.420581
x_2	0.241997	0.172980	0.323082	0.172499
x_3	0.244454	0.183782	0.316040	0.165906
x_4	0.246723	0.170095	0.315358	0.178835

Feature Importance: Results

- Recall $E[y \mid x_1, z] = -\frac{1}{2}x_1 + z$ However, we don't observe z -- instead have 3 indepedent noisy observations x_2, x_3, x_4. Trying to estimate $E[y \mid x_1, \cdots, x_4]$

```
In [31]: hide_code_in_slideshow()
         sns.set_context('notebook',font_scale=2)
         fig, ax = plt.subplots(figsize=(12,8))
         plot = imp.set_index('Feature').plot(kind='bar', ax=ax)
```



- What are the implications, and what can we learn from this experiment?

Partial Dependence Plots

- Imagine we have a subset of features we think are important.
  - This could be based on "feature importance" scores or coefficients, or other reasons (i.e. prior knowledge/research questions/etc.).
  - We may want to dig deeper to explain the relationship between our predictions and these features.
  - **Question**: Why? If we have MDI feature importance scores in hand, what do we not know?

- Directionality:
  - Note in reality we probably have complex, non-monotonic relationships
  - However even if we have a monotonic relationship, or even linear, our MDI wouldn't give any indication on the direction -- obviously weights in a linear model would.
- Partial dependence plots let us dig deeper and visualize the dependence of our prediction function (i.e. predict/predict_proba) on one or two of these features.

Partial Dependence Plots: Setup

- Consider an arbitrary prediction function f learned over a training set $\mathcal{D}$.
- This dataset includes N observations y_i of a target y for $i = 1, 2, \cdots, N$, along with p features denoted $x_{i,j}$ for $j = 1, 2, \cdots, p$ and $i = 1, 2, \cdots, N$. This model generates predictions of the form:
$$\hat{y}_i = f(x_{i,1}, x_{i,2}, \cdots, x_{i,p})$$
- In the case of a single feature x_j, Friedman's partial dependence plots are obtained by computing the following average and plotting it over a useful range of x values:
$$\phi_j(x) = \frac{1}{N} \sum_{i=1}^{N} f(x_{i,1}, \cdots, x_{i,j-1}, x, x_{i,j+1}, \cdots, x_{i,p})$$

- PDPs for more than one variable are computed (and plotted) similarly.
- **Question**: What would $\phi_j(x)$ be for a linear prediction function?

Partial Dependence Plots: Setup

$$\phi_j(x) = \frac{1}{N}\sum_{i=1}^{N} f(x_{i,1}, \cdots, x_{i,j-1}, x, x_{i,j+1}, \cdots, x_{i,p})$$

- **Question**: Think about $\phi_j(x)$ -- what issues can we already anticipate?

- Imagine $P(x_j = x_{j+1}) = 1$. Then even though there is zero density where $x_j \neq x_{j+1}$, we still can evaluate $\phi_j(x)$ at $x \neq x_{i,j+1}$ for all $i \in 1, \cdots, n$.
- **Previewing what's next**: Think about the potential impact of taking the average $\frac{1}{N}\sum_{i=1}^{N}(\cdot)$

PDP Example: California Housing

- Example derived from `sklearn` PDP example, using `sklearn` utilities.
- While not shown, we first train a GBM on the California Housing dataset:

In [33]:
```
import numpy as np
import matplotlib.pyplot as plt

from mpl_toolkits.mplot3d import Axes3D

from sklearn.model_selection import train_test_split
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble.partial_dependence import plot_partial_dependence
from sklearn.ensemble.partial_dependence import partial_dependence
from sklearn.datasets.california_housing import fetch_california_housing

cal_housing = fetch_california_housing()

# split 80/20 train-test
X_train, X_test, y_train, y_test = train_test_split(cal_housing.data,
                                                    cal_housing.target,
                                                    test_size=0.2,
                                                    random_state=1)
names = cal_housing.feature_names

reg = GradientBoostingRegressor(n_estimators=200,subsample=0.5,
                                random_state=3141)
reg = reg.fit(X_train, y_train)
```

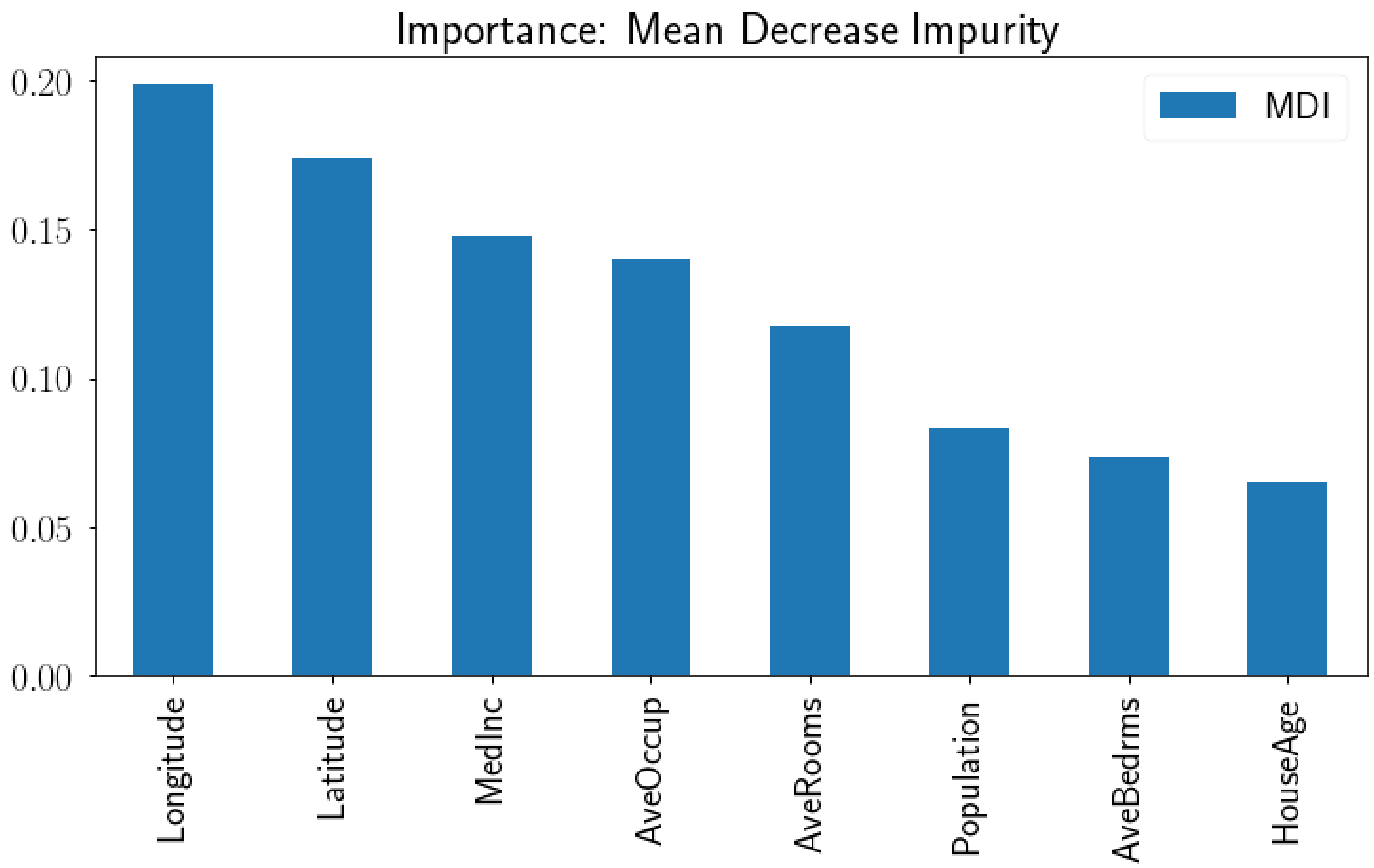
```
In [34]: hide_code_in_slideshow()
         print(cal_housing.DESCR)
```

```
California housing dataset.

The original database is available from StatLib

    http://lib.stat.cmu.edu/datasets/

The data contains 20,640 observations on 9 variables.

This dataset contains the average house value as target variable
and the following input variables (features): average income,
housing average age, average rooms, average bedrooms, population,
average occupation, latitude, and longitude in that order.

References
----------

Pace, R. Kelley and Ronald Barry, Sparse Spatial Autoregressions,
Statistics and Probability Letters, 33 (1997) 291-297.
```

PDP Example: California Housing

- Example derived from `sklearn` PDP example, using `sklearn` utilities.
- While not shown, we first train a GBM on the California Housing dataset:

```
In [35]: hide_code_in_slideshow()
         fig, ax = plt.subplots(figsize=(12,6))
         plot = pd.Series(reg.feature_importances_,
                                    index=names).rename('MDI').to_frame()\
                           .sort_values('MDI', ascending=False).plot(kind='bar',ax=ax,
                                                                  title='Importance: Mean Decrease Impurity')
```

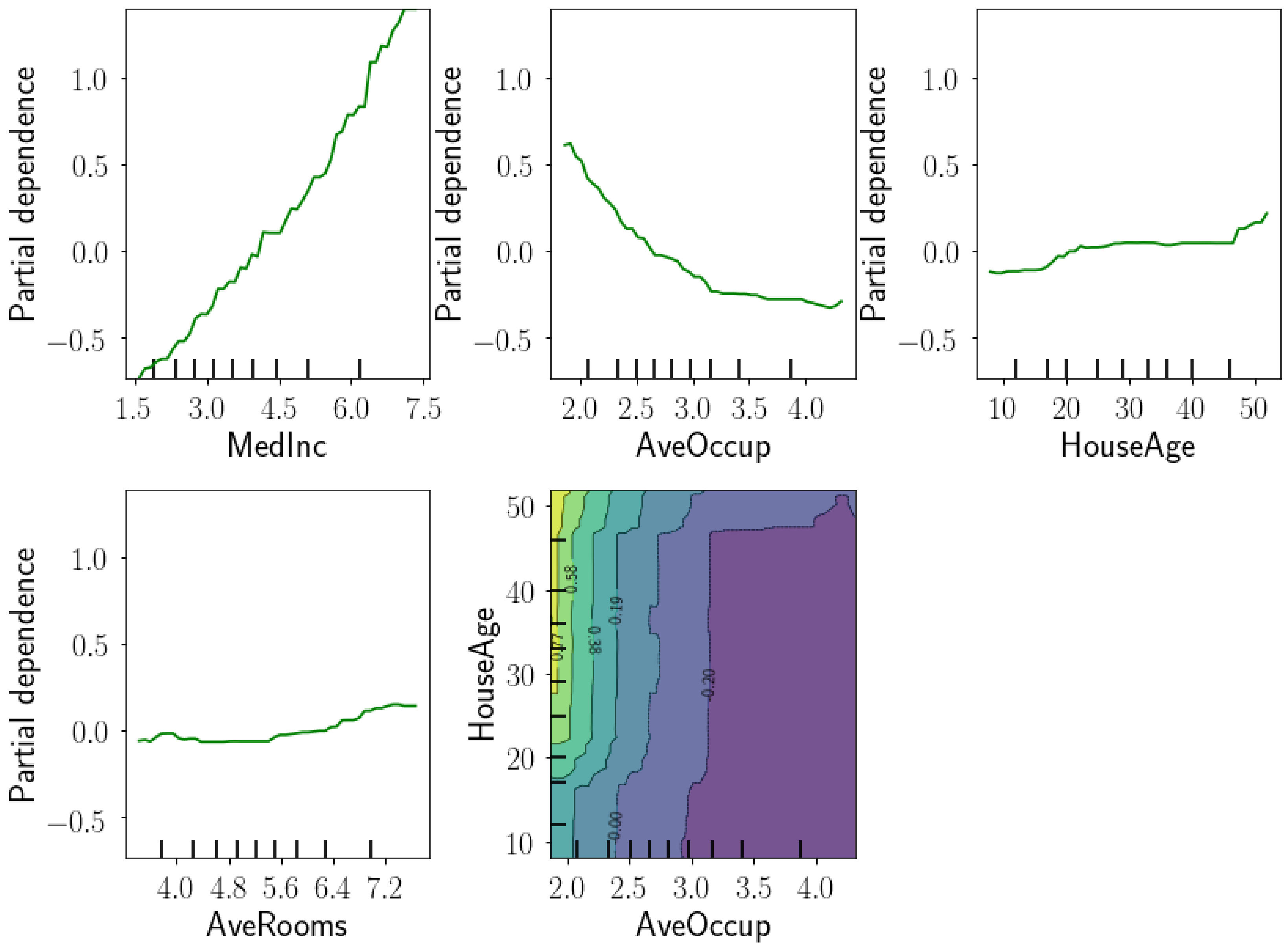


PDP Example: California Housing

- Next, we present the PDPs for several single features, and one pair of features.

```
In [36]: hide_code_in_slideshow()
         features = [0, 5, 1, 2, (5, 1)]
         fig, ax = plt.subplots(figsize=(12,10))
         fig, ax = plot_partial_dependence(reg, X_train, features,
                                           feature_names=names,
                                           n_jobs=3, grid_resolution=50,
                                           ax=ax)
         fig.suptitle('Partial dependence of house value on nonlocation features')
         plt.subplots_adjust(top=0.9)  # tight_layout causes overlap with suptitle
         plt.show()
```

Partial dependence of house value on nonlocation features



PDP Example: California Housing

- Note we don't plot the spatial features -- in fact, what would perhaps be most interesting (and a potential optional extension for indidivual exploration) would be to plot the long/lat PDP over a base map.
  - An easy python first pass might simply use `geopandas`.

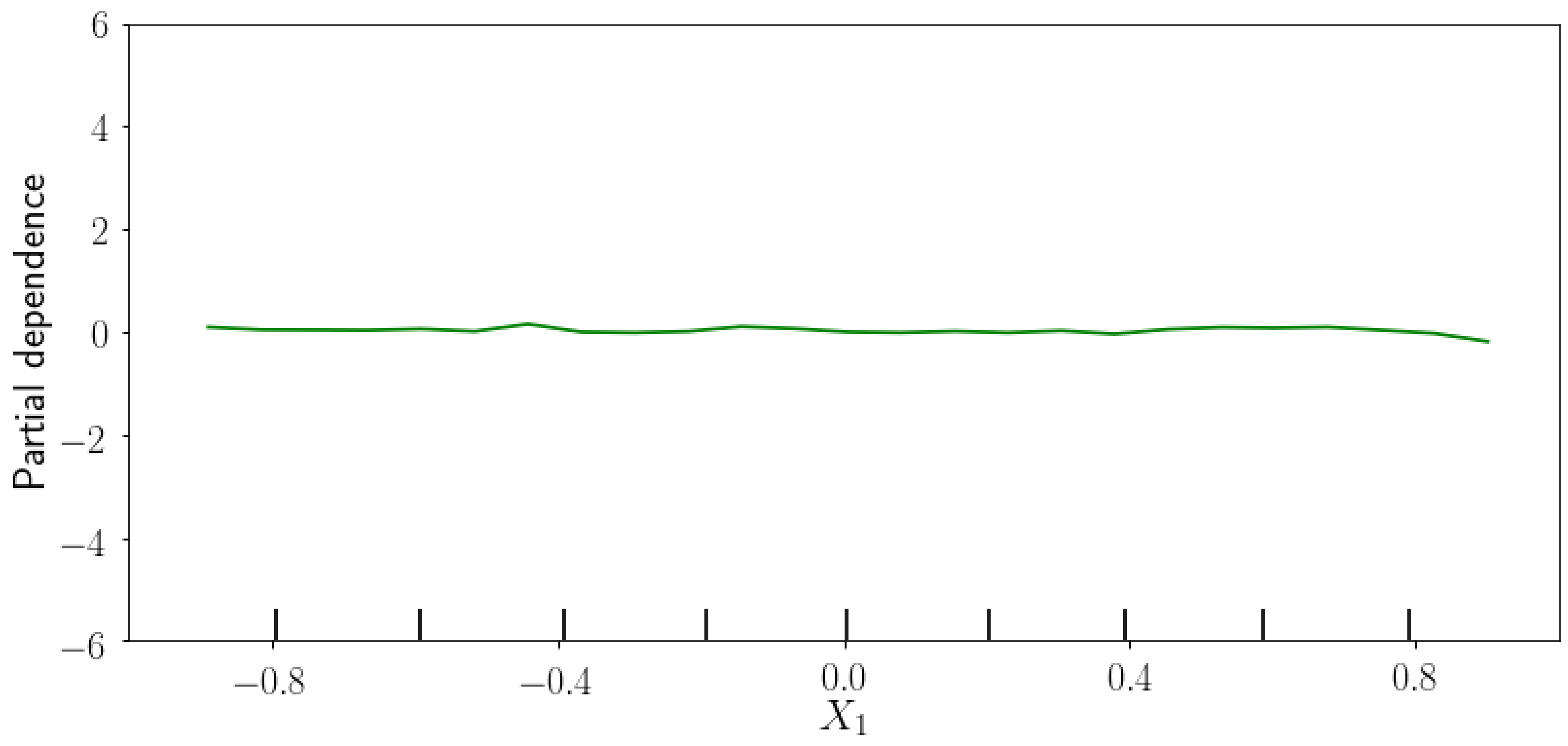
PDP Pitfalls:

- Consider the following PDP for a regression problem with $\mathcal{Y} = \mathbb{R}$ and $X = \mathbb{R}^3$.

In [37]:
```
size = 10000
X1 = np.random.uniform(-1,1,size)
X2 = np.random.uniform(-1,1,size)
X3 = np.random.uniform(-1,1,size)
eps = np.random.normal(0,0.5,size)

Y = 0.2*X1 - 5*X2 + 10*X2*np.where(X3>=0,1,0) + eps

Xs = np.stack([X1,X2,X3]).T
```

In [38]:
```
clf = GradientBoostingRegressor(max_depth=3)
params = {'n_estimators':[50,100,200]}
grid = GridSearchCV(clf, param_grid = params, n_jobs = 5, cv = 5)
grid = grid.fit(Xs,Y)
```

In [39]:
```
hide_code_in_slideshow()
fig, ax = plt.subplots(figsize=(12,8))
plot_partial_dependence(grid.best_estimator_, Xs, [1],
                        n_jobs=1, grid_resolution=25, ax=ax)
plt.xlim(-1,1)
plt.ylim(-6,6)
plt.xlabel('$X_1$')

pass
```



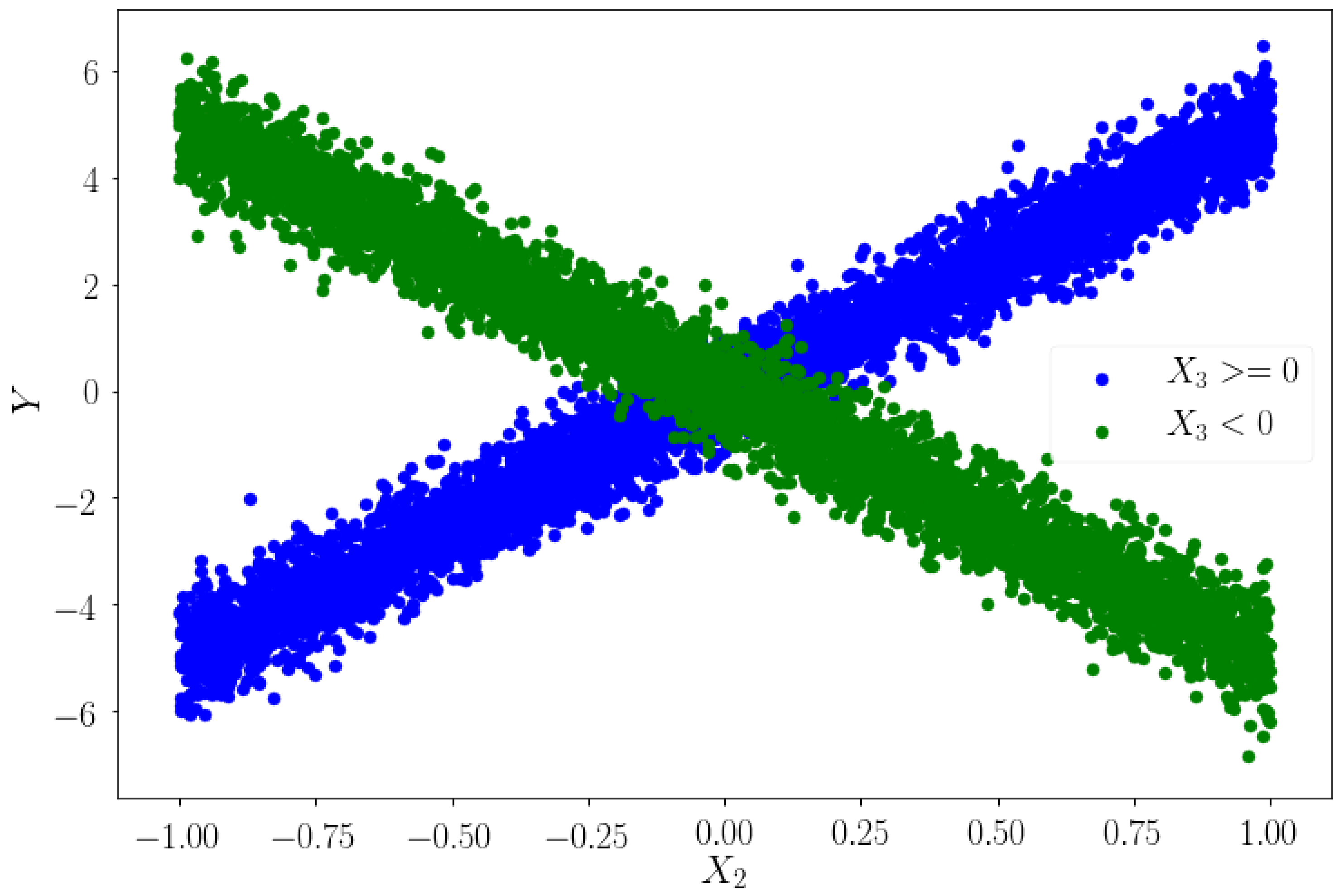
- **Question**: What can we learn about the relationship between feature X_2 and our target Y?

PDP Pitfalls:

- Here was the data generating process:

In [40]:
```
size = 10000
X1 = np.random.uniform(-1,1,size)
X2 = np.random.uniform(-1,1,size)
X3 = np.random.uniform(-1,1,size)
eps = np.random.normal(0,0.5,size)
Y = 0.2*X1 - 5*X2 + 10*X2*np.where(X3>=0,1,0) + eps

Xs = np.stack([X1,X2,X3]).T
```

In [41]:
```
hide_code_in_slideshow()
fig, ax = plt.subplots(figsize=(12,8))
plt.scatter(X2[X3>=0], Y[X3>=0], color='blue', label='$X_3>=0$')
plt.scatter(X2[X3<0], Y[X3<0], color='green', label='$X_3<0$')
plt.ylabel('$Y$')
plt.xlabel('$X_2$')
plt.legend()
plt.show()
```



PDP Pitfalls:

- Recall
$$y = 0.2x_1 - 5x_2 + 10x_2 \mathbb{1}(x_3 >= 0) + \varepsilon$$
- **Question**: Why does the PDP fail to reveal the dependence of y on x_2?

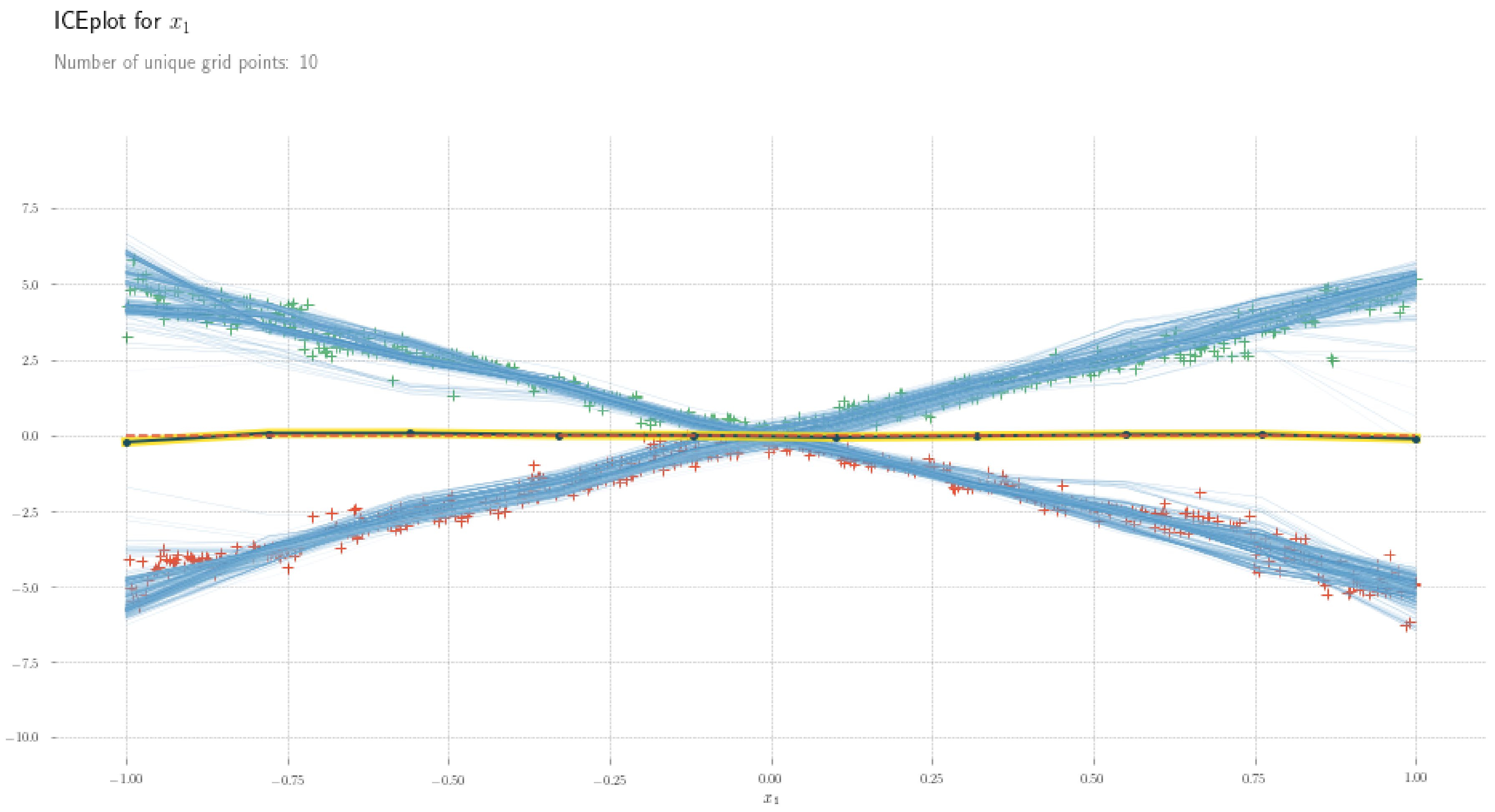
In his gradient boosting paper, Friedman identified this issue (here presented in our notation):

- In general, the functional form of $\phi_j(x)$ will depend on the particular values chosen for $\backslash j$. If, however, this dependence is **not to strong** than the average function can represent a useful summary of the partial dependence of f on the chosen variable subset j.

PDP Pitfalls: Another option

- One response to this shortcoming has been development of "Individual Conditional Expectation" plots -- see Goldstein et al, 2014 (https://arxiv.org/pdf/1309.6392.pdf).
- Their insight was that taking an average is a post-processing step that can mask structure.
- We'll use the `SauceCat/PDPbox` (https://github.com/SauceCat/PDPbox) implementation.

```
In [42]: hide_code_in_slideshow()
         from pdpbox import pdp

         train = pd.DataFrame(Xs)
         train.columns = [str(x) for x in train.columns]

         pdp_one = pdp.pdp_isolate(grid, train, '1')
         pdp.pdp_plot(pdp_one, '$x_1$',
                      plot_org_pts=True, plot_lines=True,
                      center=False, frac_to_plot=1000)
```



- **Question**: Note the average (i.e. classic PDP plot) is shown in yellow. How do the additional traces aide clarify the dependence of y on x_1 ?

Next steps

- We started by talking about feature importance.
    - This gave a set of methods for trying to build insight into how much each feature contributed to the prediction function -- *though we saw this is somewhat ill-defined.* It didn't give insight into even the directionality of simple linear relationships -- let alone more complex stucture.

- Next we looked at PDPs
    - PDPs give some insight into average relationship between one or two predictors and the target. However, this was shown to be potentially misleading, if the average relationship masks interactions.

- This led us to ICEplots, which plot a trace for each data instance separately.

- Note this trajectory (moving from global to data-instance-specific measures of importance) could be extended -- next steps might look at additive feature attribution methods such as SHAP values (https://arxiv.org/pdf/1705.07874.pdf).

Bibliography

Papers

- Brieman, L (2001). *Random Forests*. (https://link.springer.com/content/pdf/10.1023/A:1010933404324.pdf)
- Friedman, J (2001). *Greedy Function Approximation: A Gradient Boosting Machine*. (https://statweb.stanford.edu/~jhf/ftp/trebst.pdf)
- Goldstein *et al* (2014). *Peeking Inside the Black Box: Visualizing Statistical Learning with Plots of Individual Conditional Expectation* (https://arxiv.org/pdf/1309.6392.pdf)

Packages

- `scikit-learn/scikit-learn` (https://github.com/scikit-learn/scikit-learn)
- `TeamHG-Memex/eli5` (https://github.com/TeamHG-Memex/eli5)
- `SauceCat/PDPbox` (https://github.com/SauceCat/PDPbox)