

linear regression

In [2]:

```
%matplotlib inline
```

已知 $\{(\mathbf{x}_i, \mathbf{y}_i)\}$ (注意 \mathbf{x}_i 和 \mathbf{y}_i 可以是多维向量, multi-variable regression), 现在给定一个新的 \mathbf{x} 求其对应的 \mathbf{y} 值

线性模型中学习目标的定义:

$$\min_{\mathbf{w}} S, \quad S \equiv \sum_i [y_i - f(\mathbf{x}_i \cdot \mathbf{w})]^2$$

$x_0 \equiv 1$, \mathbf{w} 是列向量, 表征线性回归的参数, 其中 w_0 表示 bias

sklearn 中 $\mathbf{x}_i \cdot \mathbf{w} \rightarrow x_test[0] * coef_ [0] + \dots + x_test[n_features-1] * coef_ [n_features-1] + intercept_$

- 一般在数据少, feature space 维度高时, 可采用线性模型
- 常引入 Ridge 或 LASSO 正规化项

模型测评的标准: r^2 -score

$$r^2 \equiv 1 - \frac{\sum (y_i - f(\mathbf{x}_i \cdot \mathbf{w}))^2}{\sum (y_i - \bar{y})^2} \leq 1$$

(事实上 $\min S$ 和 $\max r^2$ 是完全等价的)

线性回归 (linear regression)

在 linear regression 中 $f(z) = z$

可以证明线性回归的学习目标, 对应的解是:

$$\mathbf{w} = (X^T X)^{-1} X^T Y, \quad X \text{ 是已知 feature 数据 } \mathbf{x}_i \text{ 对应的数据矩阵, } Y \text{ 是已知目标数据 } \mathbf{y}_i \text{ 对应的数据矩阵}$$

多项式回归 (polynomial regression)

和线性回归的差别仅在于, 输入 $(\mathbf{x}) \rightarrow (\mathbf{x}, \mathbf{x}^2, \dots)$ “维度上升”

逻辑回归 (logistic regression)

在 logistic regression 中

$$f(z) = \sigma(z) \equiv \frac{1}{1 + e^{-z}}, \quad y \in \{0, 1\} \quad z = 0 \text{ 对应 decision boundary}$$

example 1:

In [2]:

```
# %load scripts/LinearRegression_step02.py
import matplotlib.pyplot as plt
import numpy as np

data = np.array([[6, 7], [8, 9], [10, 13], [14, 17.5], [18, 18]])

X = data[:, :1]
y = data[:, 1:]

from sklearn.linear_model import LinearRegression

model = LinearRegression()
model.fit(X, y)

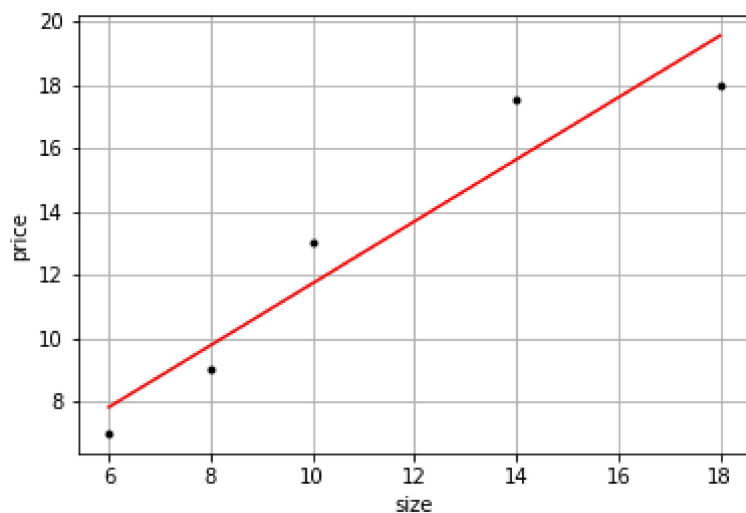
yp = model.predict(X)

score = model.score(X, y) # r-squared score

print("train score: %.6f" % score)

plt.plot(X, y, 'k.')
plt.plot(X, yp, 'r-')
plt.xlabel('size')
plt.ylabel('price')
plt.grid(True)
plt.show()
```

train score: 0.910002



example 2:

In [4]:

```
# %load scripts/LinearRegression_step03.py
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
import numpy as np

# data = np.array([[6, 7], [8, 9], [10, 13], [14, 17.5], [18, 18]])
data = np.array([[6, 4, 7], [8, 3.5, 9], [10, 6, 13], [14, 5, 17.5], [18, 3.0, 18]])

X = data[:, :2]
y = data[:, 2:]

from sklearn.linear_model import LinearRegression

model = LinearRegression()
model.fit(X, y)

yp = model.predict(X)

score = model.score(X, y) # r-squared score

print("train score: %.6f" % score)

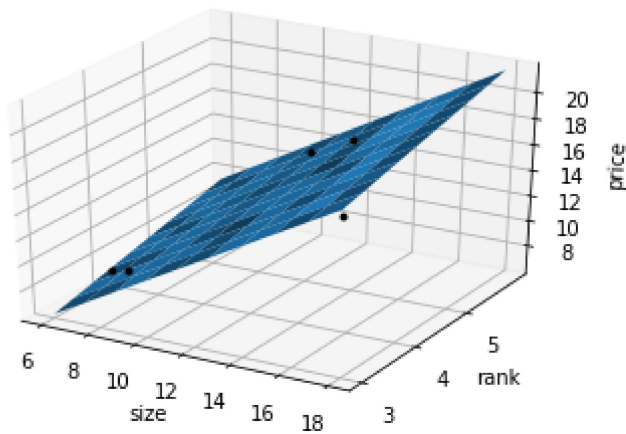
x0 = np.linspace(6, 18, 10)
x1 = np.linspace(3, 6, 10)
xx0, xx1 = np.meshgrid(x0, x1)
xx = zip(xx0.flatten(), xx1.flatten())

yp = model.predict(xx)
zz = yp.reshape((10, -1))

ax = plt.gca(projection='3d')
ax.plot(X[:,0], X[:,1], y[:,0], 'k.')
ax.plot_surface(xx0, xx1, zz)

ax.set_yticks([3, 4, 5])
ax.set_xlabel('size')
ax.set_ylabel('rank')
ax.set_zlabel('price')
plt.grid(True)
plt.show()
```

train score: 0.984400

**example 3:**

In [6]:

```
from sklearn.datasets import make_regression
from sklearn.model_selection import train_test_split

X, y, true_coefficient = make_regression(n_samples=200, n_features=30, n_informative=10, noise=100,
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=5, train_size=60)
print(X_train.shape)
print(y_train.shape)
```

```
(60L, 30L)
(60L,)
```

In [7]:

```
import numpy as np
from matplotlib import pyplot as plt
from sklearn.linear_model import LinearRegression
linear_regression = LinearRegression().fit(X_train, y_train)
print("R^2 on training set: %f" % linear_regression.score(X_train, y_train))
print("R^2 on test set: %f" % linear_regression.score(X_test, y_test))
```

```
R^2 on training set: 0.878011
R^2 on test set: 0.216332
```

In [8]:

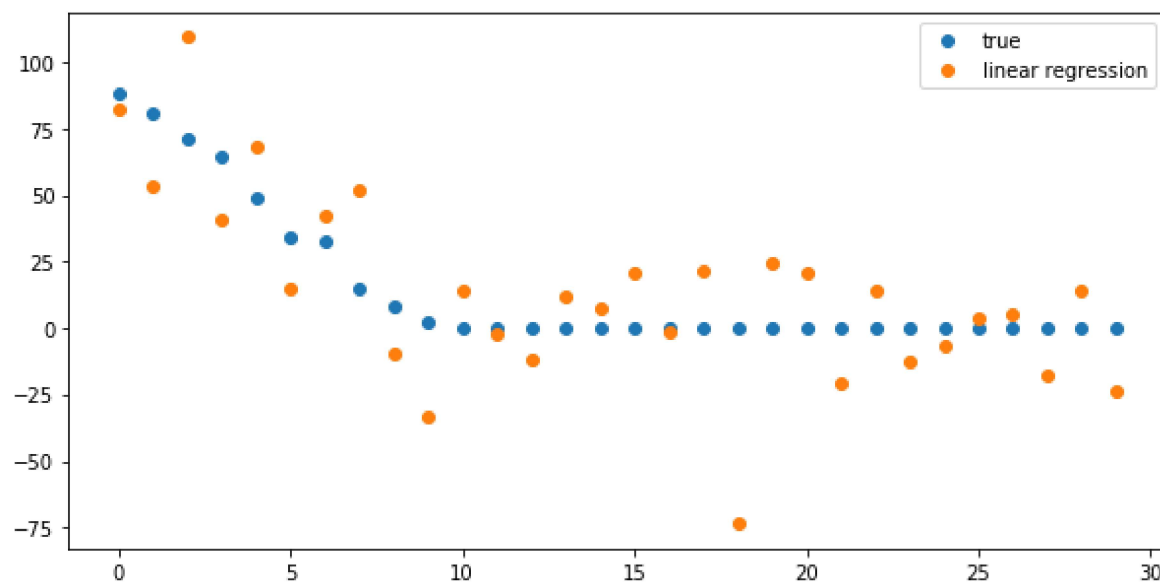
```
from sklearn.metrics import r2_score
print(r2_score(np.dot(X, true_coefficient), y))
```

```
0.598528449588
```

In [9]:

```
plt.figure(figsize=(10, 5))
coefficient_sorting = np.argsort(true_coefficient)[::-1]
plt.plot(true_coefficient[coefficient_sorting], "o", label="true")
plt.plot(linear_regression.coef_[coefficient_sorting], "o", label="linear regression")

plt.legend()
plt.show()
```



In [10]:

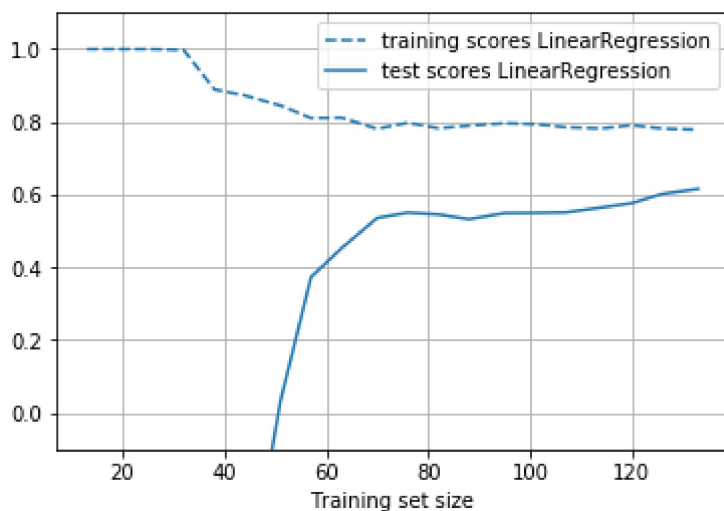
```

from sklearn.model_selection import learning_curve

def plot_learning_curve(est, X, y):
    training_set_size, train_scores, test_scores = learning_curve(est, X, y, train_sizes=np.linspace(
    estimator_name = est.__class__.__name__
    line = plt.plot(training_set_size, train_scores.mean(axis=1), '--', label="training scores " + estimator_name)
    plt.plot(training_set_size, test_scores.mean(axis=1), '-', label="test scores " + estimator_name)
    plt.xlabel('Training set size')
    plt.legend(loc='best')
    plt.grid(True)
    plt.ylim(-0.1, 1.1)

plt.figure()
plot_learning_curve(LinearRegression(), X, y)
plt.show()

```



Ridge Regression (Linear Regression with L2 regularization)

- L2 正则化
- 没有额外的计算成本（仍然是二次型）
- 超参数 α

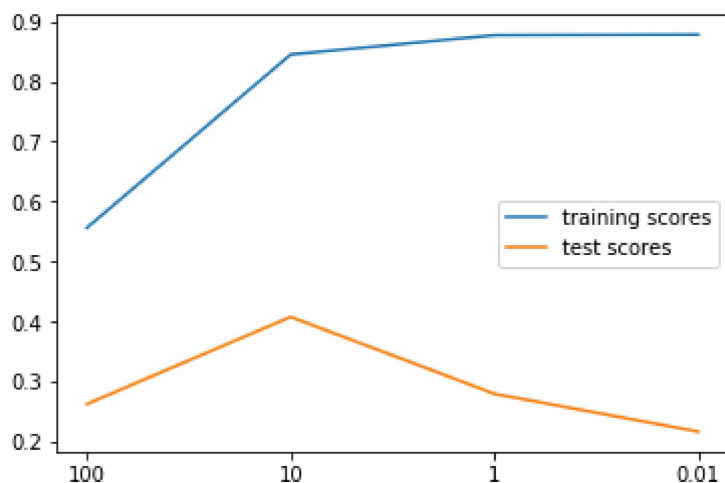
$$\min_{\mathbf{w}} S, \quad S \equiv \sum_i [y_i - f(\mathbf{x}_i \cdot \mathbf{w})]^2 + \alpha \|\mathbf{w}\|^2$$

In [19]:

```
from sklearn.linear_model import Ridge
ridge_models = {}
training_scores = []
test_scores = []

for alpha in [100, 10, 1, .01]:
    ridge = Ridge(alpha=alpha).fit(X_train, y_train)
    training_scores.append(ridge.score(X_train, y_train))
    test_scores.append(ridge.score(X_test, y_test))
    ridge_models[alpha] = ridge

plt.figure()
plt.plot(training_scores, label="training scores")
plt.plot(test_scores, label="test scores")
plt.xticks(range(4), [100, 10, 1, .01])
plt.legend(loc="best")
plt.show()
```

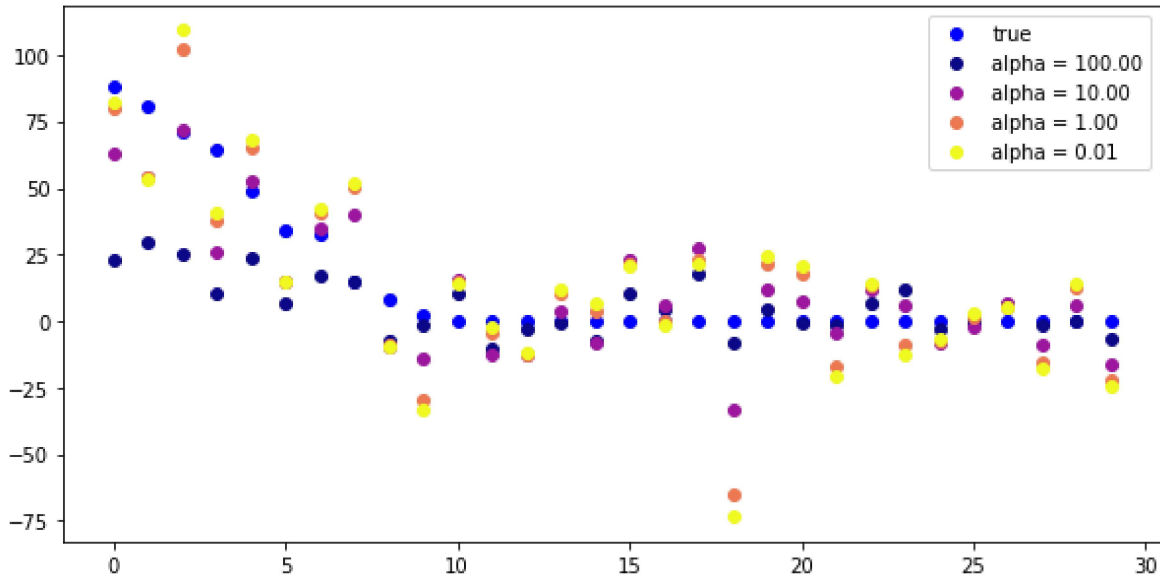


In [20]:

```
plt.figure(figsize=(10, 5))
plt.plot(true_coefficient[coefficient_sorting], "o", label="true", c='b')

for i, alpha in enumerate([100, 10, 1, .01]):
    plt.plot(ridge_models[alpha].coef_[coefficient_sorting], "o", label="alpha = %.2f" % alpha, c=plt.cm.viridis(i))

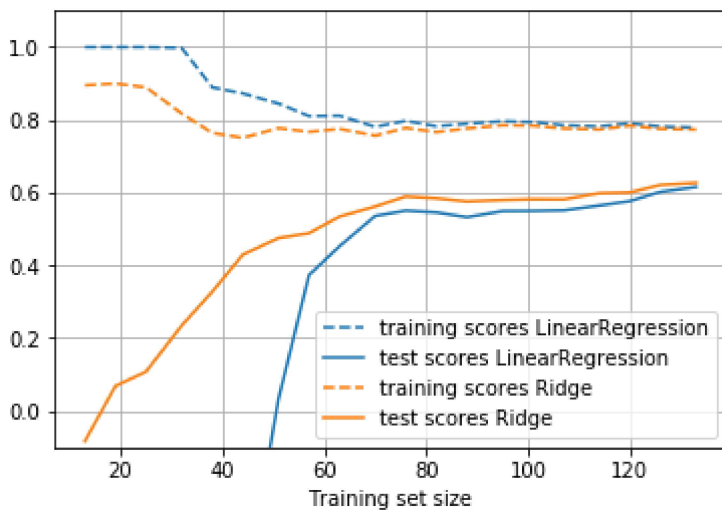
plt.legend(loc="best")
plt.show()
```



超参数 α 对 performance 的影响至关重要。

In [25]:

```
plt.figure()
plot_learning_curve(LinearRegression(), X, y)
plot_learning_curve(Ridge(alpha=10), X, y)
plt.show()
```



Lasso Regression (Linear Regression with L1 regularization)

- L1 正则化

- 可以迫使参数具有 sparsity
- 超参数 α

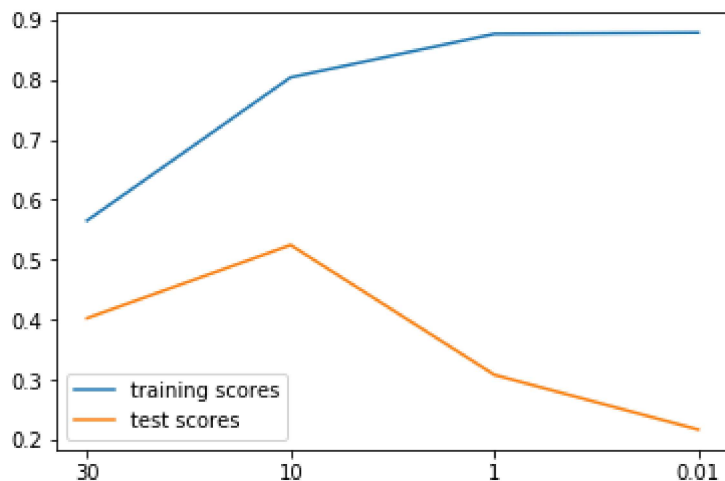
$$\min_{\mathbf{w}} S, \quad S \equiv \sum_i [y_i - f(\mathbf{x}_i \cdot \mathbf{w})]^2 + \alpha \|\mathbf{w}\|$$

In [26]:

```
from sklearn.linear_model import Lasso

lasso_models = {}
training_scores = []
test_scores = []

for alpha in [30, 10, 1, .01]:
    lasso = Lasso(alpha=alpha).fit(X_train, y_train)
    training_scores.append(lasso.score(X_train, y_train))
    test_scores.append(lasso.score(X_test, y_test))
    lasso_models[alpha] = lasso
plt.figure()
plt.plot(training_scores, label="training scores")
plt.plot(test_scores, label="test scores")
plt.xticks(range(4), [30, 10, 1, .01])
plt.legend(loc="best")
plt.show()
```

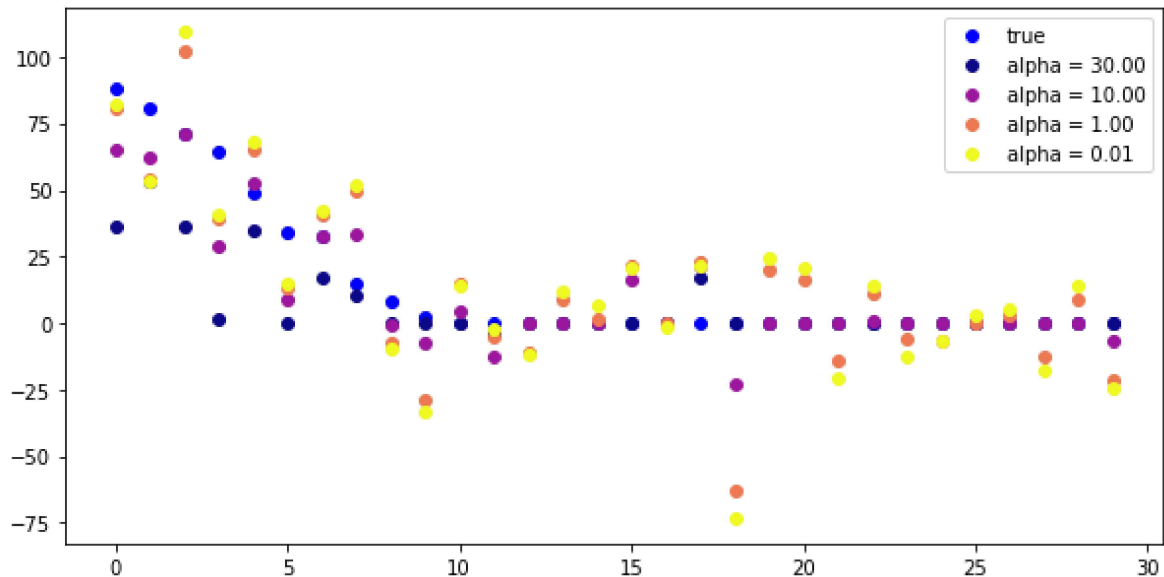


In [30]:

```
plt.figure(figsize=(10, 5))
plt.plot(true_coefficient[coefficient_sorting], "o", label="true", c='b')

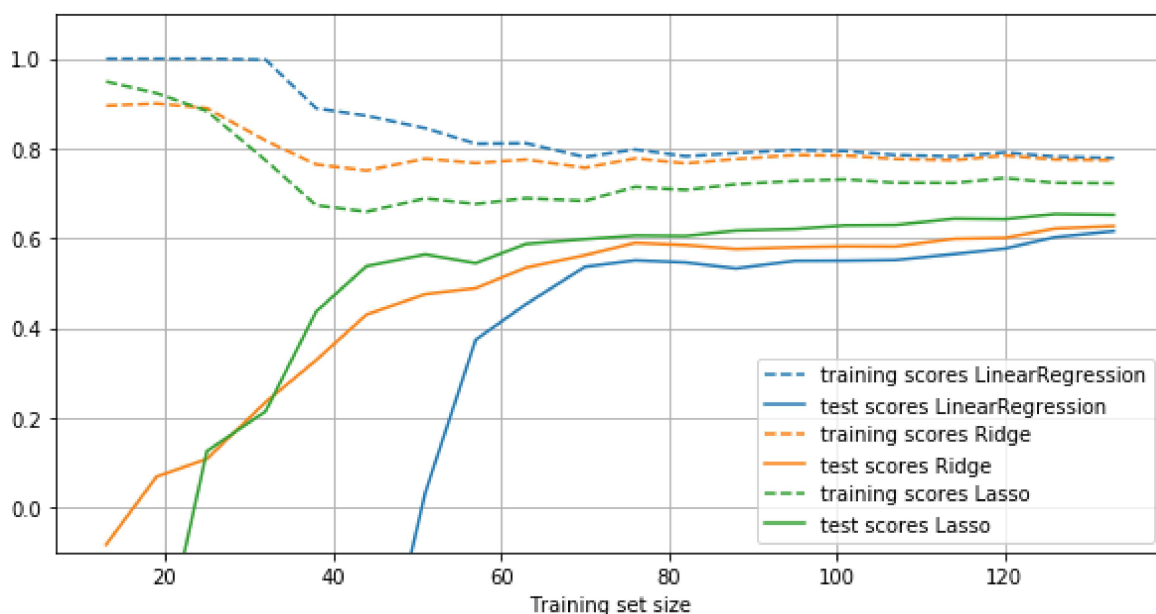
for i, alpha in enumerate([30, 10, 1, .01]):
    plt.plot(lasso_models[alpha].coef_[coefficient_sorting], "o", label="alpha = %.2f" % alpha, c=plt.cm.viridis(i))

plt.legend(loc="best")
plt.show()
```



In [33]:

```
plt.figure(figsize=(10, 5))
plot_learning_curve(LinearRegression(), X, y)
plot_learning_curve(Ridge(alpha=10), X, y)
plot_learning_curve(Lasso(alpha=10), X, y)
plt.show()
```



ElasticNet

$$\min_{\mathbf{w}} S, \quad S \equiv \sum_i [y_i - f(\mathbf{x}_i \cdot \mathbf{w})]^2 + \alpha r \|w\| + 0.5\alpha(1 - r)\|w\|^2$$