In [1]:
```
# settings
import numpy as np
import matplotlib.pylab as plt
import scipy, scipy.stats
from ipywidgets import interact, interactive, fixed
import ipywidgets as widgets
%matplotlib inline
plt.rcParams['figure.figsize'] = (8.0, 4.0)
```

\usepackage*amssymb*

3.4. Principal Component Analysis (PCA)

- The PCA is a simple standard method for dimensionality reduction
- Principal Idea: Determine a low-dimensional linear subspace that contains the largest share of the variance.

<img src = "images/projection.png" width="30%">

Given: data set $X = \{\vec{x}^{\alpha}\}_{\alpha=1\ldots N}, \vec{x}^{\alpha} \in \mathbb{R}^d$ Let w.l.o.g. the data be **centered**, i.e. all features are shifted/translated so that means are 0:

$$\frac{1}{N}\sum_{\alpha=1}^{N}\vec{x}^{\alpha} = \vec{0}$$

Approach: Maximize the variance of the data after projection onto a vector $\hat{v}$.

- The estimated variance in the subspace along vector $\hat{v}$ with $\|\hat{v}\| = 1$ is given by

$$\begin{aligned} F(\hat{v}) &= \frac{1}{N}\sum_{\alpha=1}^{N}(\vec{x}^{\alpha\tau}\hat{v})^2 \\ &= \frac{1}{N}\sum_{\alpha=1}^{N}\hat{v}^{\tau}\vec{x}^{\alpha}\vec{x}^{\alpha\tau}\hat{v} \\ &= \hat{v}^{\tau}\underbrace{\left[\frac{1}{N}\sum_{\alpha=1}^{N}\vec{x}^{\alpha}\vec{x}^{\alpha\tau}\right]}_{\text{estimated covariance matrix}C}\hat{v} \\ &= \hat{v}^{\tau}C\hat{v} \end{aligned}$$

In [7]:
```
# projection plot
R = np.random.randn(200, 2)*[5,1]
a = -np.pi/180*40
X = (np.matrix([[np.cos(a), np.sin(a)], [-np.sin(a), np.cos(a)]])*R.transpose()
).transpose()

def pltprj(alpha=0.1):
    plt.subplot(121)
    plt.plot(X[:,0], X[:,1], ".")
    vec = [np.cos(alpha), np.sin(alpha)]
    plt.plot([-10*vec[0], 10*vec[0]], [-10*vec[1], 10*vec[1]], 'r', lw=2)
    plt.axis('equal')
    plt.subplot(122)
    prj = np.zeros(np.shape(X))
    prj[:,0] = np.dot(np.matrix(X), vec)
    prj[:,1] = np.dot(np.matrix(X), [-np.sin(alpha), np.cos(alpha)])
    # plt.plot(prj[:,0], prj[:,1], ".")
    plt.plot(prj[:,0], 0*prj[:,0], ".")
    plt.axis([-15, 15, -10, 10]);
    # plt.axis('equal')

interact(pltprj, alpha=(0, np.pi, 0.05));
```

- C is a positive semi-definite symmetric matrix.
- Thus it exists a decomposition

$$C = UDU^\tau$$

with

- $U = [\vec{u}_1, \dots, \vec{u}_d]$ being the matrix of eigenvectors of C and
- $D = \mathrm{diag}(\lambda_1, \dots, \lambda_d)$: are the real-valued eigenvalues of C.

Wanted:

$$\sigma^2_{\max} = \max_{\vec{w}} F(\vec{w}) = \max \frac{\vec{w}^\tau C \vec{w}}{\vec{w}^\tau \vec{w}}$$

Method: Determine the zero crossings of all partial derivatives of $F(\vec{w})$

$$\nabla_{\vec{w}} F = \frac{2C\vec{w}}{\vec{w}^\tau \vec{w}} - \frac{\vec{w}^\tau C \vec{w}}{(\vec{w}^\tau \vec{w})^2} 2\vec{w} = 0$$

- Note that here the product rule $(uv)' = u'v + uv'$ has been applied
- We can reshape the equation as

$$C\vec{w} = \underbrace{\left[\frac{\vec{w}^\tau C \vec{w}}{\vec{w}^\tau \vec{w}}\right]}_{C\hat{w} \quad = \quad \lambda} \vec{w} \quad \Big| \quad \text{then multiply eq. with} \quad \cdot 1/\|\vec{w}\| \quad \hat{w}$$

- Yet this is just the eigenvalue condition!
- The necessary condition of stationarity leads to solutions that are the eigenvectors
- For that reason F is maximized by the eigenvector belonging to the largest eigenvalue

Usually we use a sorted order or eigenvalues: $\lambda_1 \geq \lambda_2 \geq \dots \lambda_d \ (\geq 0)$.

Then we can simply write

$$F_{\max} = \sigma^2_{\max} = \lambda_1$$

With that, we can determine the first principal component of the data:

$$y_1^\alpha = \hat{u}_1^\tau \vec{x}^\alpha \qquad \text{(projection indices)}$$

Transformation back into data space:

$$\tilde{x}^\alpha = \hat{u}_1 y_1^\alpha = \underbrace{\hat{u}_1 \hat{u}_1^\tau}_{\text{Projektionsmatrix}} \vec{x}^\alpha \text{ (reconstruction)}$$

Concerning the data compression

- Coding using equation 'projection indices'
- Decoding using equation 'reconstruction'

The estimated variance along the first principal component is $\sigma_1^2 = \lambda_1$

Total variance of the data distribution:

$$\begin{aligned} V &= \sum_{j=1}^{d} \text{Var}(x_j) = \frac{1}{N} \sum_{\alpha=1}^{N} \vec{x}^{\alpha\tau} \vec{x}^\alpha \quad \text{(since mean 0)} \\ &= \frac{1}{N} \sum_\alpha \text{trace}(\vec{x}^\alpha \vec{x}^{\alpha\tau}) \\ &= \text{trace}\left[\frac{1}{N} \sum_\alpha \vec{x}^\alpha \vec{x}^{\alpha\tau} \right] \\ &= \text{trace}(C) \end{aligned}$$

But since $C = UDU^\tau$ and $\text{trace}(M) = \text{trace}(U^\tau M U) \ \forall \ U$ orthonormal, it is

$$V = \text{trace}(D) = \text{trace}(\text{diag}(\lambda_1, \dots, \lambda_d)) = \sum_{i=1}^{d} \lambda_i$$

Iterative application to perpendicular subspace

Now we search the 1-dimensional subspace which contains the largest fraction of the remaining variance $\sum_{i=2}^{d} \lambda_i$.

The decomposition yields for the orthogonal part

$$\vec{x} = \vec{x}^{(1)} + (\vec{x} - \vec{x}^{(1)}) = \hat{u}_1 \hat{u}_1^\tau \vec{x} + \underbrace{(I - \hat{u}_1 \hat{u}_1^\tau)}_{\text{projection matrix}} \vec{x}$$

Now we maximize

$$\begin{aligned} F^{(2)}(v) &= \frac{1}{N} \sum_\alpha^N \hat{v}^\tau \left[(I - \hat{u}_1 \hat{u}_1^\tau) \vec{x}^\alpha \right] \left[(I - \hat{u}_1 \hat{u}_1^\tau) \vec{x}^\alpha \right]^\tau \hat{v} \\ &= \frac{1}{N} \sum_\alpha^N \hat{v}^\tau (I - \hat{u}_1 \hat{u}_1^\tau) \vec{x}^\alpha \vec{x}^{\alpha\tau} (I - \hat{u}_1 \hat{u}_1^\tau) \hat{v} \\ &= \hat{v}^\tau (I - \hat{u}_1 \hat{u}_1^\tau) C (I - \hat{u}_1 \hat{u}_1^\tau) \hat{v} \\ &= \hat{v}^\tau (C - \hat{u}_1 \hat{u}_1^\tau C - C \hat{u}_1 \hat{u}_1^\tau + \hat{u}_1 \hat{u}_1^\tau C \hat{u}_1 \hat{u}_1^\tau) \hat{v} \\ &= \hat{v}^\tau (C - \hat{u}_1 \lambda_1 \hat{u}_1^\tau - \underbrace{\lambda_1 \hat{u}_1 \hat{u}_1^\tau + \hat{u}_1 \lambda_1 \hat{u}_1^\tau}_{=0}) \hat{v} \\ &= \hat{v}^\tau (C - \lambda_1 \hat{u}_1 \hat{u}_1^\tau) \hat{v} \\ &= \hat{v}^\tau \left[UDU^\tau - U \text{diag}(\lambda_1, 0, 0 \dots, 0) U^\tau \right] \hat{v} \\ &= \hat{v}^\tau \left[U \text{diag}(0, \lambda_2, \lambda_3 \dots, \lambda_d) U^\tau \right] \hat{v} \\ &= \hat{v}^\tau \tilde{C} \hat{v} \end{aligned}$$

We see:

- the solution is analog to finding the first principal component. The optimal vector now belongs to the largest eigenvalue of $\tilde{C}$, and thus is λ_2.
- Thus $\hat{v}_2 = \hat{u}_2$ is the direction of the 2nd principal component with variance $\sigma_2^2 = \lambda_2$
- In analogy, we obtain all further components as

$$\hat{v}_j = \hat{u}_j \ , \ \sigma_j^2 = \lambda_j \ \ \forall \ j = 1, \dots, d$$

Remarks:

- Principal components are uncorrelated!

$$\begin{aligned} \text{corr}(y_j, y_k) &= \frac{1}{N} \sum_{\alpha} \hat{u}_j^\tau \vec{x}^\alpha \cdot \hat{u}_k^\tau \vec{x}^\alpha \\ &= \hat{u}_j^\tau C \hat{u}_k = \lambda_k \underbrace{\hat{u}_j^\tau \hat{u}_k}_{=0 \ \forall j \neq k} \end{aligned}$$

- The eigenvectors are pairwise orthogonal

[ws17EOT20171206]

Summary (PCA, general case of uncentered data sets):

1. Compute the estimated covariance matrix $\hat{C}$ of the data set $X = \{\vec{x}^\alpha\}_{\alpha=1,\dots,N}$

$$\hat{C} = \frac{1}{N-1}\sum_{\alpha=1}^{N}(\vec{x}^\alpha - \bar{x})(\vec{x}^\alpha - \bar{x})^\tau \quad \text{(symmetric } d \times d\text{-matrix)}$$

2. Compute the eigenvalues λ_j and eigenvectors $\hat{u}_j$ of $\hat{C}$:

$$\hat{C}\hat{u}_j = \lambda_j \hat{u}_j$$

Since $\hat{C}$ is symmetric, $\hat{u}_i^\tau \hat{u}_j = \delta_{ij}$ can always be achieved.
Then it holds:

a. Each data vector $\vec{x}^\alpha$ can be decomposed into its Eigenvector decomposition

$$\vec{x}^\alpha = \bar{x} + \sum_{j=1}^{d} y_j^\alpha \hat{u}_j\,, \qquad \text{(eigenvalue decomposition)}$$

where the coefficients y_j^α are given by

$$y_j^\alpha = \hat{u}_j^\tau(\vec{x}^\alpha - \bar{x}) \qquad \text{(projection indices)}$$

b. y_j^α are centered (i.e. mean 0) and pairwise uncorrelated and the eigenvalues λ_i are the variances of the component:

$$\frac{1}{N-1}\sum_\alpha y_i^\alpha y_j^\alpha = \lambda_i \delta_{ij}$$

c. The matrix $\hat{C}$ can be represented by

$$\hat{C} = U\hat{D}U^\tau$$

- where $U = (\hat{u}_1, \dots, \hat{u}_d)$ has the eigen vectors as columns,
- and $\hat{D} = \mathrm{diag}(\lambda_1, \dots, \lambda_d)$ is a diagonal matrix of the eigenvalues

Proof:

a) follows from inserting the definitions

b)

$$\begin{aligned}
\frac{1}{N-1}\sum_\alpha y_i^\alpha y_j^\alpha &= \frac{1}{N-1}\sum_\alpha (\hat{u}_i \cdot (\vec{x}^\alpha - \bar{x}))\cdot(\hat{u}_j \cdot (\vec{x}^\alpha - \bar{x})) \\
&= \frac{1}{N-1}\sum_\alpha \hat{u}_i^\tau((\vec{x}^\alpha - \bar{x})(\vec{x}^\alpha - \bar{x})^\tau \hat{u}_j \\
&= \hat{u}_i^\tau \hat{C}\hat{u}_j \\
&= \hat{u}_i^\tau \lambda_j \hat{u}_j \\
&= \delta_{ij}\lambda_j
\end{aligned}$$

c) is equivalent to $U^\tau \hat{C} U = \mathrm{diag}(\lambda_1, \dots, \lambda_d)$.

- The ij element of this equation is the last bit of the equation string of (b).

Interpretation:

- The eigenvector decomposition describes each data point (vector) by a new parameter vector $\vec{y}^\alpha = (y_1^\alpha, \dots, y_d^\alpha)$.
- The $\vec{y}^\alpha$ are obtained by a linear transformation from the $\vec{x}^\alpha$. However, the features are now pairwise uncorrelated. (yet not independent!!!)
- The eigenvalues λ_j equal the variance of the respective component y_j^α.

Relevance for Dimensionality reduction:

W.l.o.g. let all eigenvectors be enumerated so that the eigenvalues form a descending series:

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d \geq 0$$

Then stopping the decomposition after the q-th term yields:

$$\tilde{\vec{x}}^{\alpha} = \bar{x} + \sum_{j=1}^{q} y_j^{\alpha} \hat{u}_j$$

with approximation error

$$\vec{\delta}_{\alpha} = \sum_{j=q+1}^{d} y_j^{\alpha} \hat{u}_j.$$

Note that this is the smallest possible approximation error when using only q components!

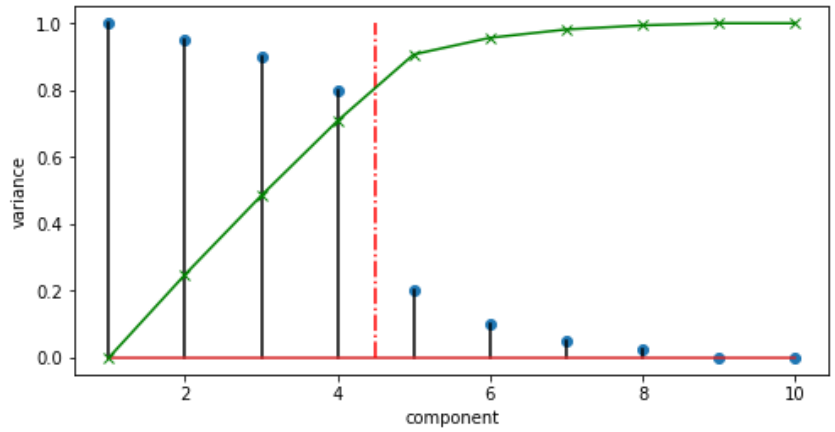
The vector $\tilde{\vec{x}}^{\alpha}$ can be regarded as orthogonal projection of $\vec{x}^{\alpha}$ on the q-dimensional subspace $\mathrm{span}\{\hat{u}_j | j = 1, \ldots, q\}$.

The total variance $\hat{\sigma}^2$ of $\vec{\delta}_{\alpha}$ over all data is

$$\begin{aligned}
\hat{\sigma}^2 &= \frac{1}{N-1} \sum_{\alpha} \vec{\delta}_{\alpha}^2 \\
&= \frac{1}{N-1} \sum_{i>q} \sum_{\alpha} \hat{u}_i^T \hat{u}_i (y_i^{\alpha})^2 \\
&= \frac{1}{N-1} \sum_{i>q} \sum_{\alpha} 1 \cdot (y_i^{\alpha})^2 \\
&= \sum_{i>q} \left(\frac{1}{N-1} \sum_{\alpha} (y_i^{\alpha})^2 \right) \\
&= \sum_{i>q} \lambda_i
\end{aligned}$$

- That means that the expected approximation error is equal to the sum of the eigenvalues belonging to the unused eigenvectors.
- Using the q largest eigenvalues (i.e. projection on $\mathrm{span}\{\hat{v}_j \mid j = 1, \ldots, q\}$) thus minimizes the mean squared error (MSE) among all linear projections onto a q-dimensional linear subspace (called *Karhunen-Loeve-expansion*)
- Choice of q: best according to the eigenvalue distribution of $\hat{C}$.

In [10]:
```
lambdas = [1, 0.95, 0.9, 0.8, 0.2, 0.1, 0.05, 0.025, 0.0, 0.0]
cdf = [np.sum(lambdas[:d]) for d in np.arange(len(lambdas))]
ii = np.arange(len(lambdas))+1
plt.stem(ii, lambdas, "k-")
plt.plot([4.5, 4.5], [0,1], "r-.")
plt.plot(ii, cdf/max(cdf), "gx-")
plt.xlabel("component"); plt.ylabel("variance");
```



- Eigenvalue analysis provides important information about the intrinsic data dimensionality
- intrinsic dimensionality can of course be much lower!

Remarks:

- Eigenvalue analysis is purely variance-driven
- no statement is made about the semantic content in the dimension
- non-linear structures are 'by principle' not findable using PCA
- Few large eigenvalues can maybe only contain useless noise...
- Practical procedure requires particular tricks if very-high-dimensional data are given
  - e.g. images where d may be up to 10^6.