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)
```

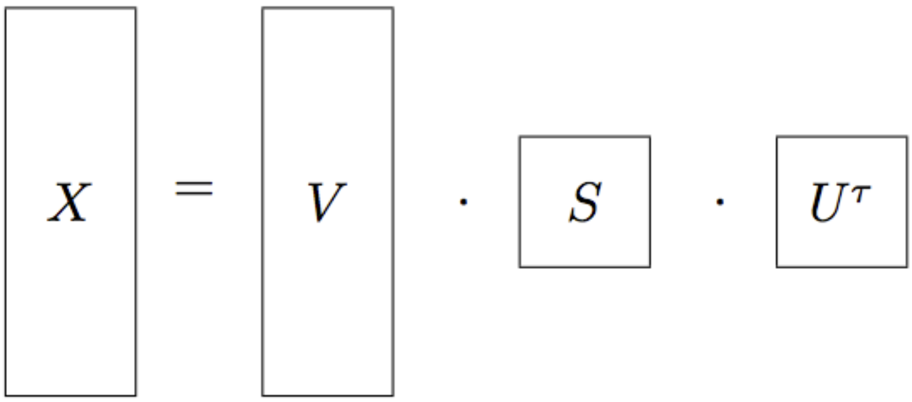
\usepackage*amssymb*

3.6 PCA via Singular Value Decomposition (SVD)

Singular Value Decomposition (SVD) allows an efficient computation of the PCA, so to say: PCA in a single execution step.

The SVD of a $N \times d$ matrix X finds the decomposition into a product of three matrices

$$X = VSU^\tau \,,$$



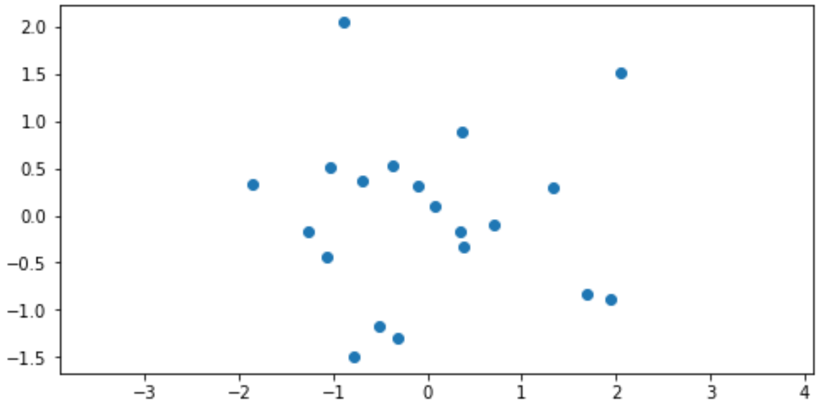
where

$$\begin{aligned} U &= d \times d\text{-orthogonal matrix} \\ S &= \mathrm{diag}(s_1, \ldots, s_d) \text{ diagonal matrix of singular values of } X \\ V &= \text{Matrix of } d \text{ pairwise orthonormal columns} \in \mathbb{R}^N \end{aligned}$$

For the PCA we here take as input the **centered** data matrix $X = (\vec{x}^1, \ldots, \vec{x}^\alpha)^\tau$ and interprete the decomposition as follows:

1. The columns $\hat{u}_i$ of U are the eigenvectors of the covariance matrix $\hat{C}$ of the data
   - because
   $$(N-1)\hat{C} = \sum_{\alpha=1}^{N} \vec{x}^\alpha \vec{x}^{\alpha\tau} = X^\tau X = US\underbrace{V^\tau V}_{I_d}SU^\tau = US^2U^\tau$$
   - Since $\hat{C}$ has the eigenvalue decomposition $\hat{C} = U\hat{D}U^\tau$, it is immediately obvious that in addition it is $\lambda_i = s_i^2/(N-1)$.
   - Note: if the mean is not estimated from the data, we can use N instead of $N-1$.
2. The kth column of matrix $V \cdot S$ contains the projection indices for the kth principal component
   $$y_k^\alpha = \hat{u}_k^\tau \vec{x}^\alpha = \vec{x}^{\alpha\tau} \hat{u}_k = V_{\alpha k} S_{kk}$$
   - Reordering the SVD-equation gives $XU = VS$ and thus directly the above statement.

In [12]:
```
# create mean-centered data
N, dim = 20, 3
data = np.random.randn(N, dim)
data = data - np.mean(data, 0)
plt.plot(data[:,0], data[:,1], 'o'); plt.axis('equal');
```



In [18]:
```
# compute SVD
u, s, vh = np.linalg.svd(data, full_matrices=False)
print("singualar values", np.sort(s))
```

```
singualar values [ 3.6657852   4.50154667  5.02182538]
```

In [19]:
```
# compute eigenvalues via C and diag
C = np.cov(data.T)
eigvals, eigvecs = np.linalg.eig(C)
print("eigenvalues:", np.sort(eigvals))
```

```
eigenvalues: [ 0.70726216  1.06652223  1.32730159]
```

In [26]:
```
# check difference with the 1/(N-1) normalization
print("difference is approx. 0:", np.sort(eigvals) - np.sort(s)**2/(N-1))
```

```
difference is approx. 0: [ -3.33066907e-16  -2.22044605e-16   4.44089210e-16]
```