Mining and Processing Biomedical Data

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Matrix completion techniques

Matrix completion for biomedical tasks

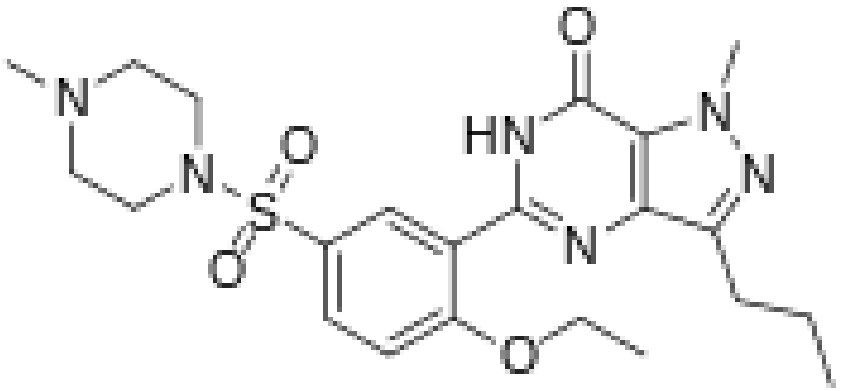
- Drug-target prediction
- Prediction of side effects of drugs
- Link prediction in biological networks
- Analysis of DNA-methylation in case of cancerous tissues

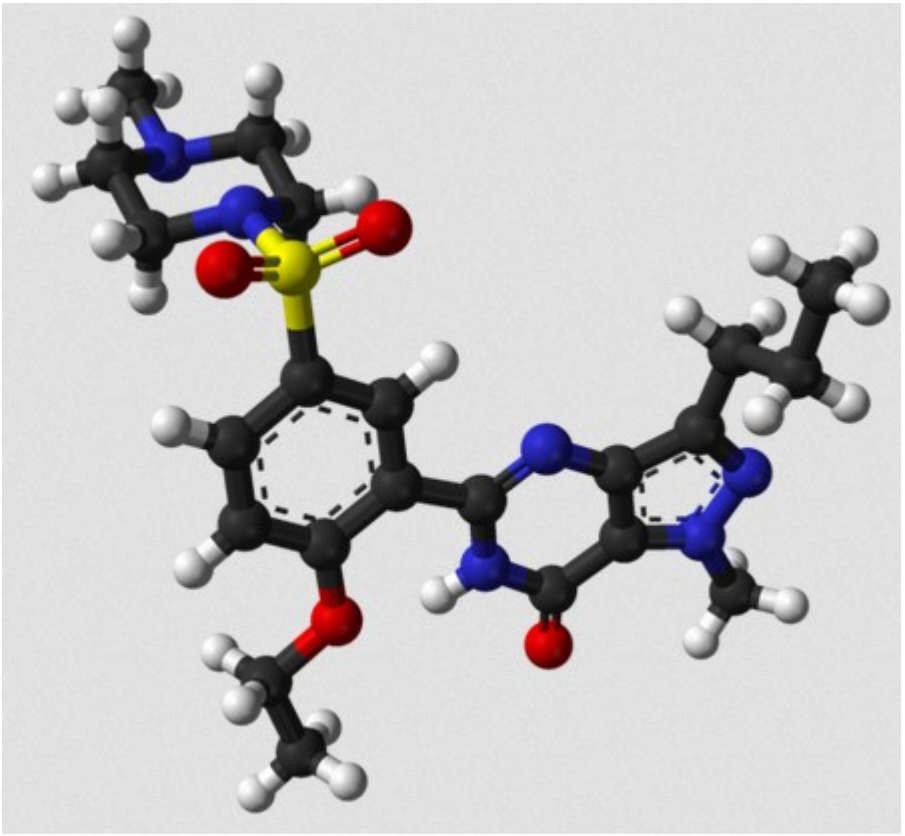
Module overview

- Lecture 3A – Motivation, „side effect“ of Viagra
- Lecture 3B – Matrix multiplication
- Lecture 3C – Matrix factorisation (MF) based on the minimization of sum of squared errors with gradient descent
- Lecture 3D – Link prediction
- Lecture 3E – Restricted Boltzmann Machines (RBMs)
- Lecture 3F – Drug-target prediction with RBMs, MF for the analysis of DNA-methylation

Example: „side effects“ of Viagra (Sildenafil)

See also http://en.wikipedia.org/wiki/Sildenafil





Lessons learned from the example

- Some side effects of a drug may potentially not be discovered during clinical trials
  - e.g. because these side effects are only present under certain conditions
- The side effect of a drug may be even more relevant than the effect the drug was designed to have
- Computational methods may predict potential side effects

Prediction of drug-target interactions

- Assume that we are given a drug. This drug is unlikely to interact with a randomly selected target, e.g., probability of the interaction is 0.1%.
- Due to the **large amount** of possible targets, the expected value of the number of interactions may be in the order of dozens!
- Computational methods for drug-target interaction may generate useful hypothesises about which drug-target interactions should be tested.

Multiplication of matrices

Example:
Multiplication of 2x2 matrices

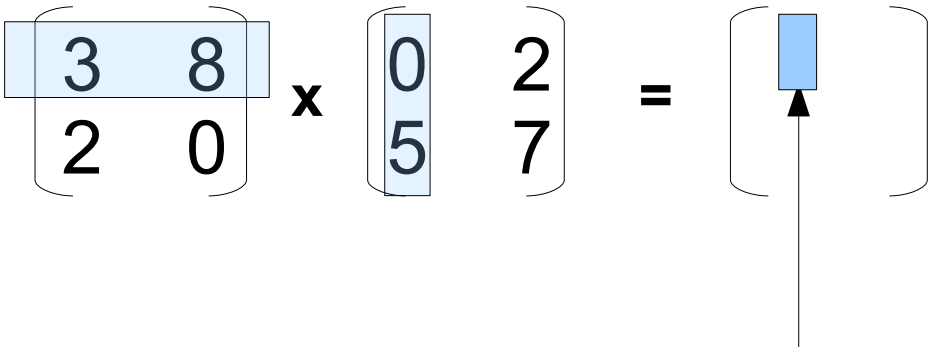
$$\begin{pmatrix} 3 & 8 \\ 2 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 2 \\ 5 & 7 \end{pmatrix}$$

Example:
Multiplication of 2x2 matrices

$$\begin{pmatrix} 3 & 8 \\ 2 & 0 \end{pmatrix} \times \begin{pmatrix} 0 & 2 \\ 5 & 7 \end{pmatrix} = \begin{pmatrix} & \\ & \end{pmatrix}$$

Example: Multiplication of 2x2 matrices

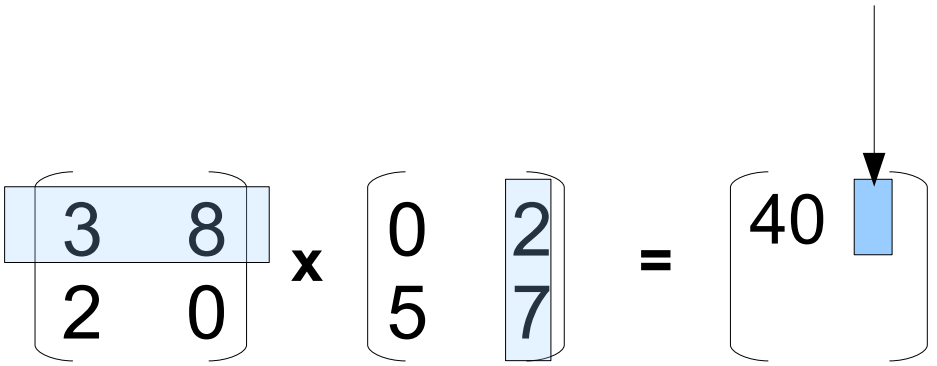
„row times column“



(3 x 0) + (8 x 5) = 0 + 40 = 40

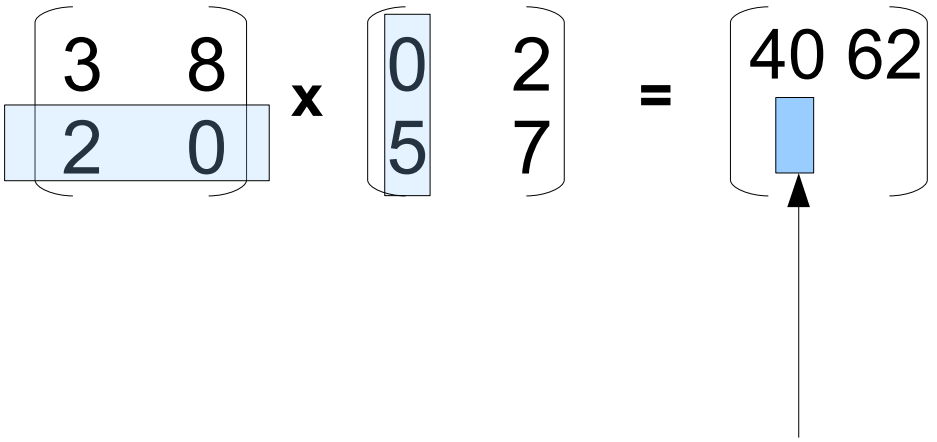
Example:
Multiplication of 2x2 matrices

„row times column“ (3 x 2) + (8 x 7) = 6 + 56 = 62



Example: Multiplication of 2x2 matrices

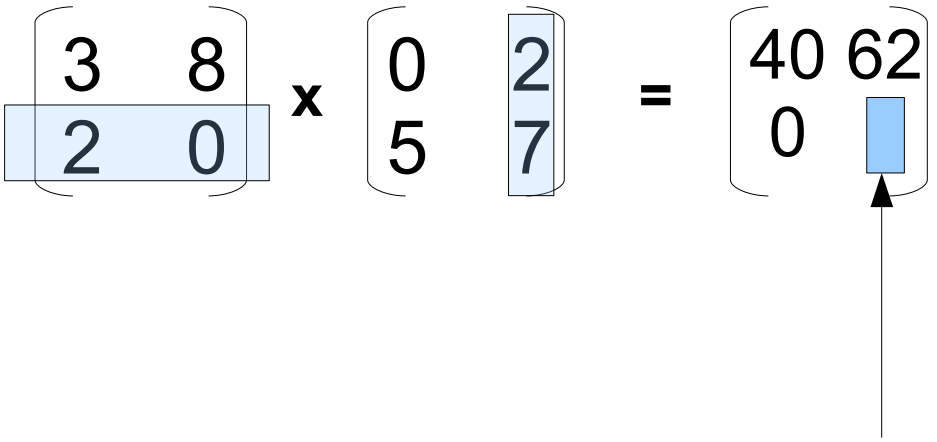
„row times column“



(2 x 0) + (0 x 5) = 0 + 0 = 0

Example: Multiplication of 2x2 matrices

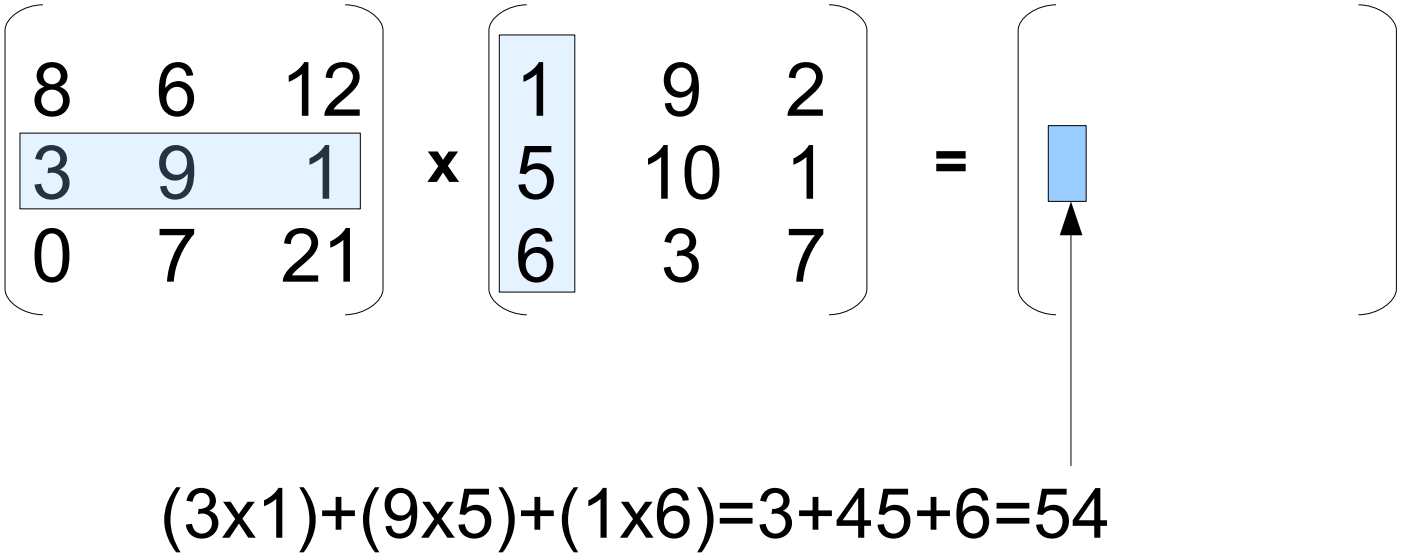
„row times column“



(2 x 2) + (0 x 7) = 4 + 0 = 4

Example: Multiplication of 3x3 matrices

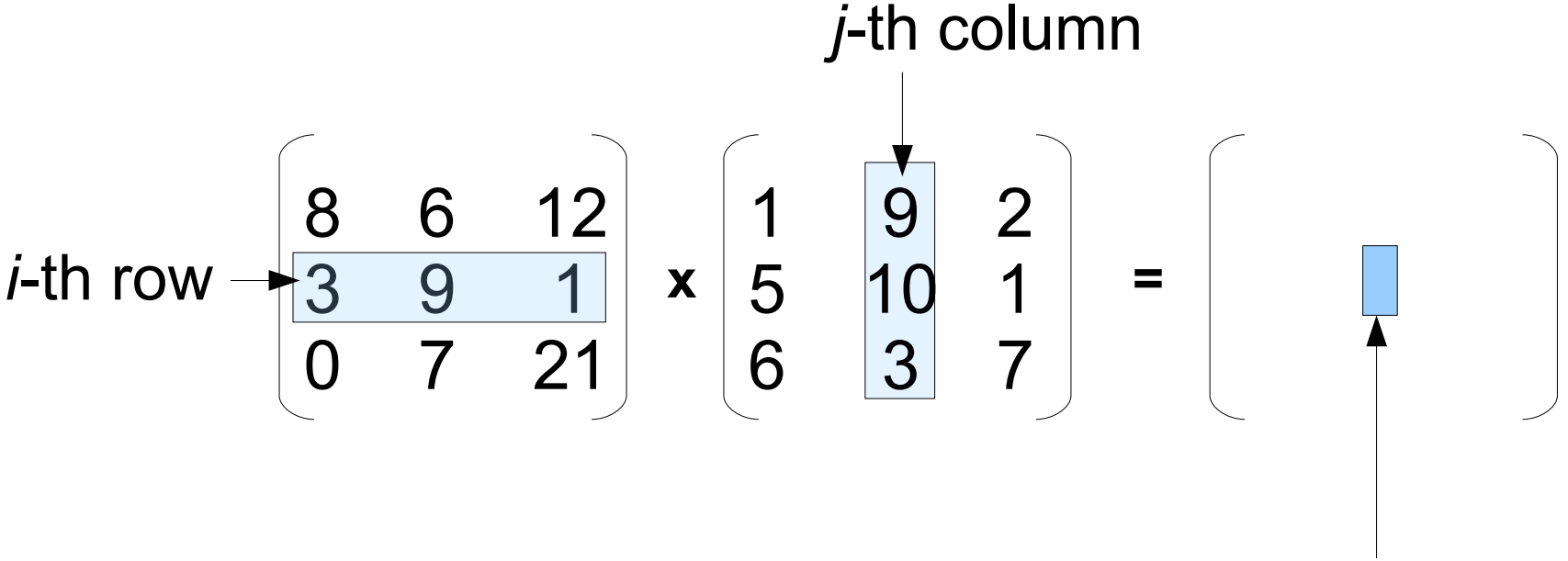
„row times column“



(3x1)+(9x5)+(1x6)=3+45+6=54

Example: Multiplication of 3x3 matrices

„row times column“



Element in the *i*-th row and *j*-th column:
product of the *i*-th row of the first matrix
and the *j*-th column of the second matrix