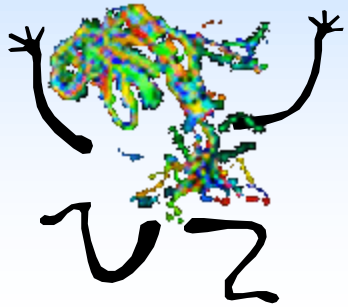
GET THAT PROTEIN!



Eller

TDDE49

Databaser och informationssäkerhet för bioinformatik

http://www.ida.liu.se/~TDDE49

Lärare

- Examinator: Olaf Hartig
- FÖ: Olaf Hartig, Ulf Kargén, Patrick Lambrix
- LA: Adriana Concha, Ulf Kargén
- projekt: Patrick Lambrix, Adriana Concha
- databasadministration: Adriana Concha

- studierektor: Patrick Lambrix

- Olaf/ Adriana på engelska

Kurslitteratur

- Elmasri, R. and Navathe, S. B. Fundamentals of Database Systems, Addison Wesley.
- (Padron-McCarthy, webbkurs på Svenska)
- van Oorschot P: Computer Security and the Internet.
- Anderson R, Security Engineering.
- Adam Shostack: Threat Modeling.
- Lab + projekt: på hemsidan

Databaser

- Ett (av flera) sätt att lagra data i elektronisk format
- Används i det vardagliga livet: bank, bokning av hotell eller resa, sökning i biblioteket, handla
- nyare tillämpningar: multimediadatabaser, geografiska informationssystem, realtiddatabaser

Databaser

- databashanteringssystem (DBMS): en uppsättning program som tillåter en användare att skapa och underhålla en databas
- databassystem = databas + databashanteringssystem

Bioinformatik

- Kända sekvenser samlas i en stor databas. Insamlande och studier av sekvenser och jämförelser av sekvensernas uppbyggnad i olika organismer kallas bioinformatik. Forskningen inom bioinformatik är beroende av avancerad datalogi och matematik. (forksningsrådens strategidokument 2000)

Bioinformatik

- Bioinformatics: research, development, or application of computational tools and approaches for expanding the use of biological, medical, behavioral or health data, including those to acquire, store, organize, archive, analyze or visualize data. (National Institutes of Health)

Bioinformatik

Ämnen på ISMB:

- protein structure and modeling
- sequence motifs, alignments and families
- networks and modeling
- gene structure, regulation and modeling
- sequence and phylogeny
- databases, information and knowledge management

TDDE49 Databaser och informationssäkerhet för Bioinformatik

- Denna kurs: fokus på biologiska databanker

Relation med andra kurser inom TB-programmet:

- förkunskaper: molekylärbiologi, programmering
- bioinformatik

Årets ändringar i kursen

Inga större ändringar

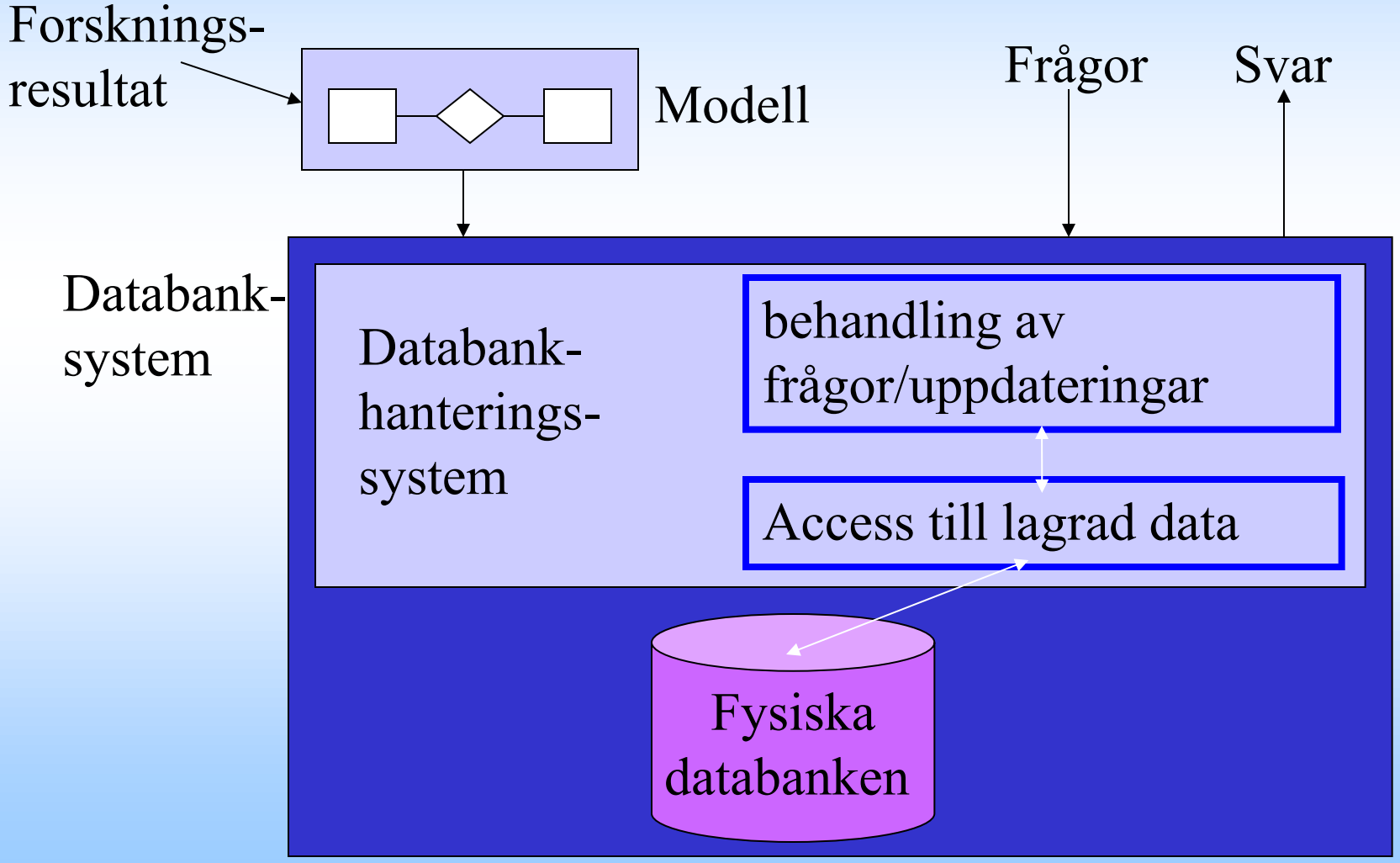
Tidigare ändringar senaste åren:

- Namnbyte
- Informationssäkerhet tillkommer
- Information retrieval, semi-strukturerad data, teoretiska delar av relationsdatabaser utgår.
- Nya labbar för databasdelen.
- Flipped classroom för databasföreläsningarna.

Biologiska databanker

- biologisk data i elektronisk format
- exempel: SWISS-PROT/UniProt, EMBL, DDBJ, PDB, GENBANK, KEGG, ACEDB
- används dagligen i forskningen

Biologiska databanker



Frågeställningar

- Vilken information lagrar man?
- Hur lagras informationen? (hög och låg nivå)
- Hur accessar man informationen?
  (användarnivå, systemnivå)
- Hur återställer man en databank efter crash?
- Hur kan flera användare accessa och uppdatera informationen samtidigt?

Personer

- databankadministratör
- databankdesigner
- användare (’end user’)
- programmerare av tillämpningar

- DBMS designer
- utvecklare av verktyg
- operator, underhåll

1 tgctacccgc gcccgggctt ctggggtgtt ccccaaccac ggcccagccc tgccacaccc
61 cccgcccccg gcctccgcag ctcggcatgg gcgcgggggt gctcgtcctg ggcgcctccg
121 agcccggtaa cctgtcgtcg gccgcaccgc tccccgacgg cgcggccacc gcggcgcggc
181 tgctggtgcc cgcgtcgccg cccgcctcgt tgctgcctcc cgccagcgaa agccccgagc
241 cgctgtctca gcagtggaca gcgggcatgg gtctgctgat ggcgctcatc gtgctgctca
301 tcgtggcggg caatgtgctg gtgatcgtgg ccatcgccaa gacgccgcgg ctgcagacgc
361 tcaccaacct cttcatcatg tccctggcca gcgccgacct ggtcatgggg ctgctggtgg
421 tgccgttcgg ggccaccatc gtggtgtggg gccgctggga gtacggctcc ttcttctgcg
481 agctgtggac ctcagtggac gtgctgtgcg tgacggccag catcgagacc ctgtgtgtca
541 ttgccctgga ccgctacctc gccatcacct cgcccttccg ctaccagagc ctgctgacgc
601 gcgcgcgggc gcggggcctc gtgtgcaccg tgtgggccat ctcggccctg gtgtccttcc
661 tgcccatcct catgcactgg tggcgggcgg agagcgacga ggcgcgccgc tgctacaacg
721 accccaagtg ctgcgacttc gtcaccaacc gggcctacgc catcgcctcg tccgtagtct
781 ccttctacgt gcccctgtgc atcatggcct tcgtgtacct gcgggtgttc cgcgaggccc
841 agaagcaggt gaagaagatc gacagctgcg agcgccgttt cctcggcggc ccagcgcggc
901 cgccctcgcc ctcgccctcg cccgtccccg cgcccgcgcc gccgcccgga cccccgcgcc
961 ccgccgccgc cgccgccacc gccccgctgg ccaacgggcg tgcgggtaag cggcggccct
1021 cgcgcctcgt ggccctacgc gagcagaagg cgctcaagac gctgggcatc atcatgggcg
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1141 agctggtgcc cgaccgcctc ttcgtcttct tcaactggct gggctacgcc aactcggcct
1201 tcaaccccat catctactgc cgcagccccg acttccgcaa ggccttccag ggactgctct
1261 gctgcgcgcg cagggctgcc cgccggcgcc acgcgaccca cggagaccgg ccgcgcgcct
1321 cgggctgtct ggcccggccc ggacccccgc catcgcccgg ggccgcctcg gacgacgacg
1381 acgacgatgt cgtcggggcc acgccgcccg cgcgcctgct ggagccctgg gccggctgca
1441 acggcggggc ggcggcggac agcgactcga gcctggacga gccgtgccgc cccggcttcg
1501 cctcggaatc caaggtgtag ggcccggcgc ggggcgcgga ctccgggcac ggcttcccag
1561 gggaacgagg agatctgtgt ttacttaaga ccgatagcag gtgaactcga agcccacaat
1621 cctcgtctga atcatccgag gcaaagagaa aagccacgga ccgttgcaca aaaaggaaag
1681 tttgggaagg gatgggagag tggcttgctg atgttccttg ttg

DEFINITION	Homo sapiens adrenergic, beta-1-, receptor
ACCESSION	NM_000684
SOURCE ORGANISM	human
REFERENCE	1
AUTHORS	Frielle, Collins, Daniel, Caron, Lefkowitz, Kobilka
TITLE	Cloning of the cDNA for the human beta 1-adrenergic receptor
REFERENCE	2
AUTHORS	Frielle, Kobilka, Lefkowitz, Caron
TITLE	Human beta 1- and beta 2-adrenergic receptors: structurally and functionally related receptors derived from distinct genes

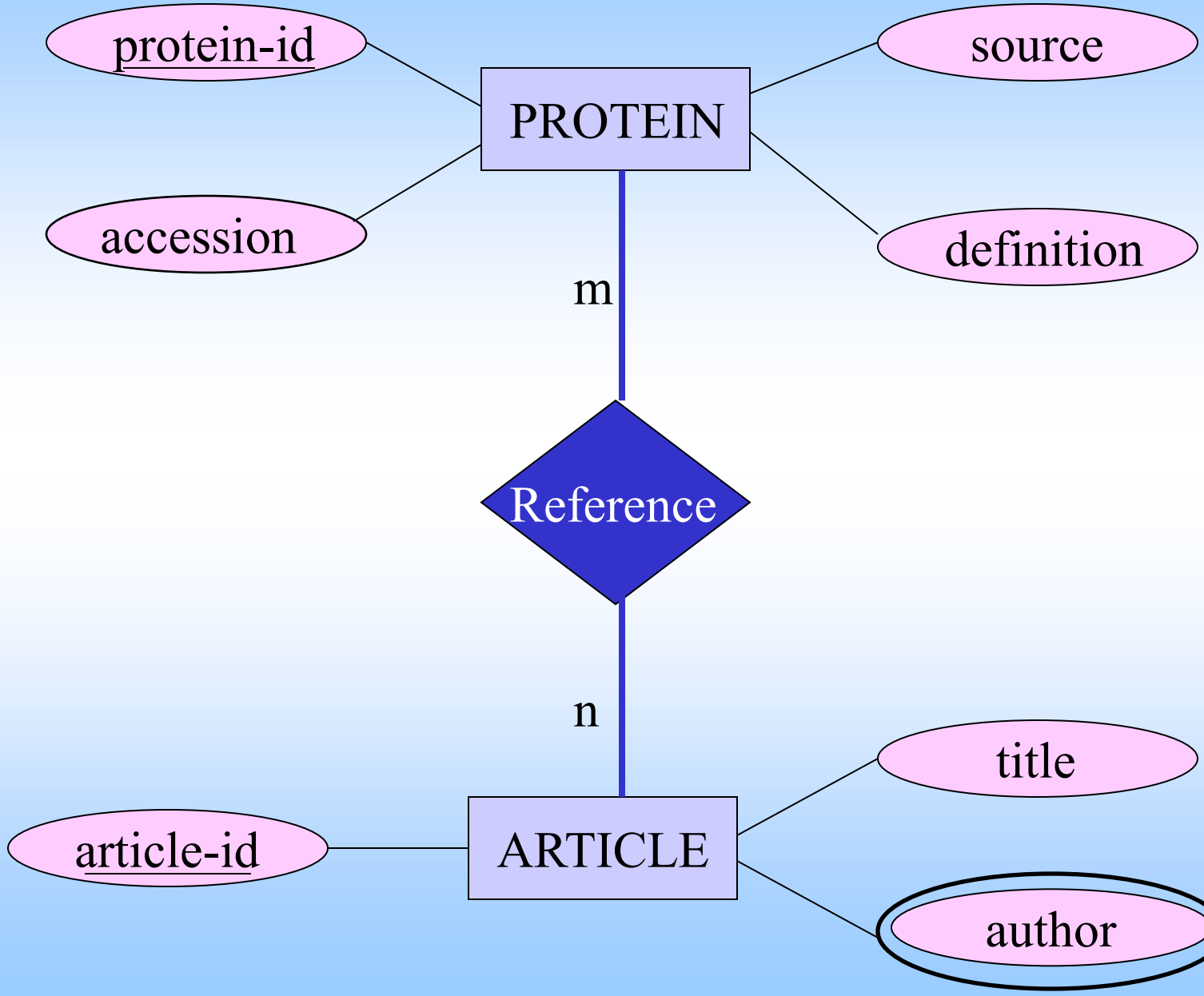
Vilken information lagrar man?

- Modell av verkligheten
  - Entity-Relationship modell (ER)
  - Unified Modeling Language (UML)

Entity-Relationship

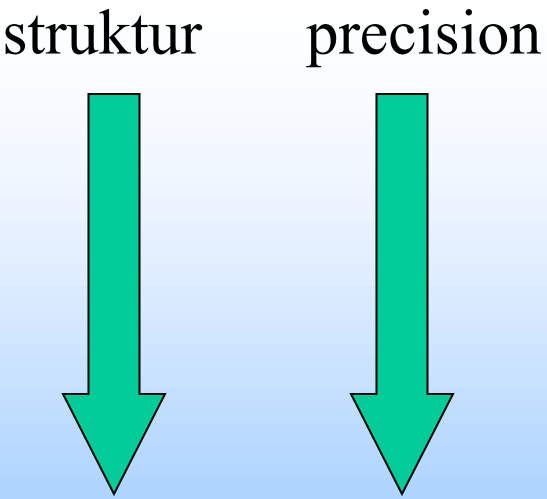
- entiteter och attribut
- entitetstyper
- nyckelattribut
- relationer
- kardinalitetsvillkor

Entity-relationship



Hur lagras informationen? (hög nivå) Hur accessar man informationen? (användarnivå)

- Text (IR)
- Semistrukturerad data
- Datamodeller (DB)
- Regler + Fakta (KB)



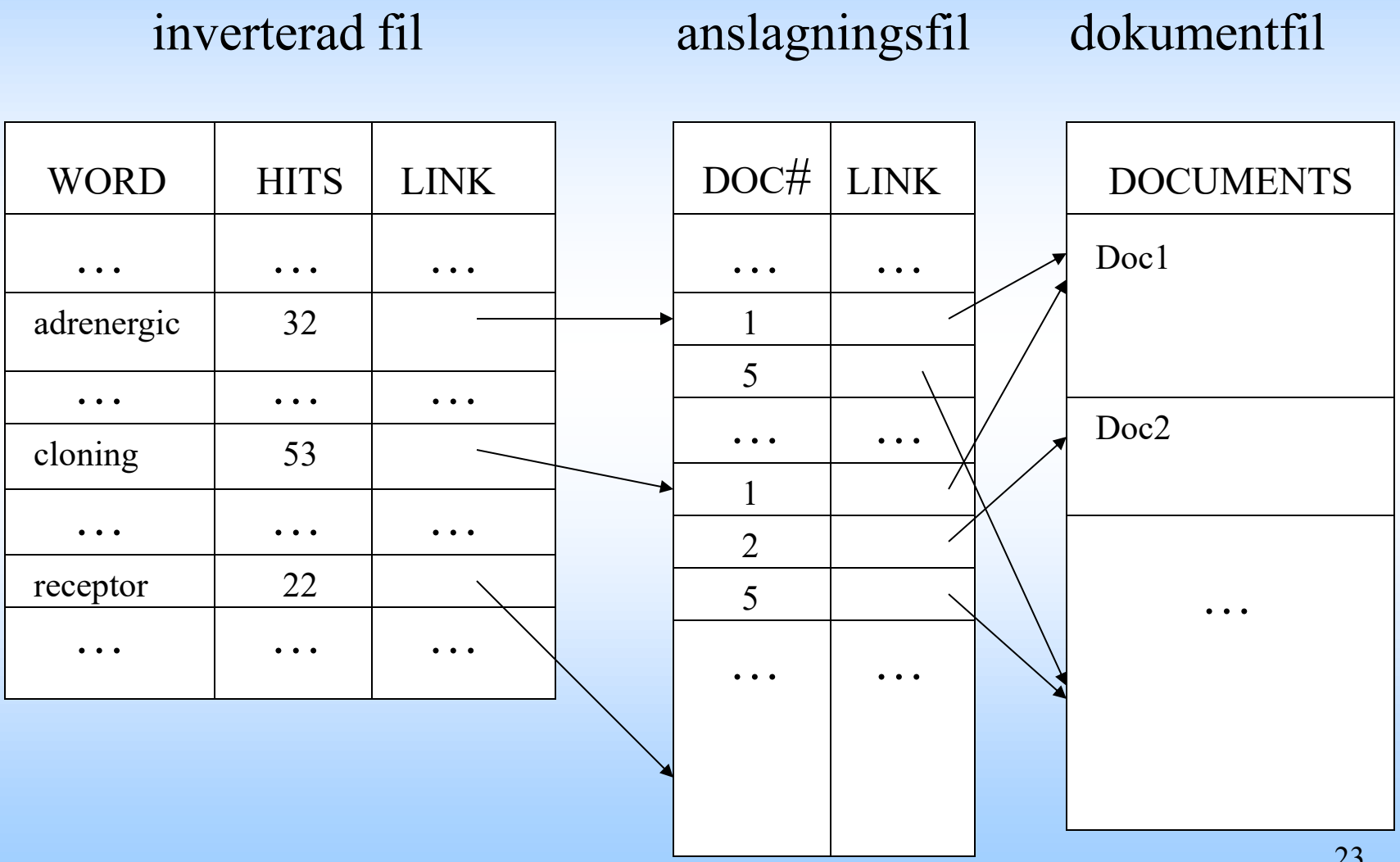
Text - Information Retrieval

- sökning baseras på ord
- konceptuella modeller:

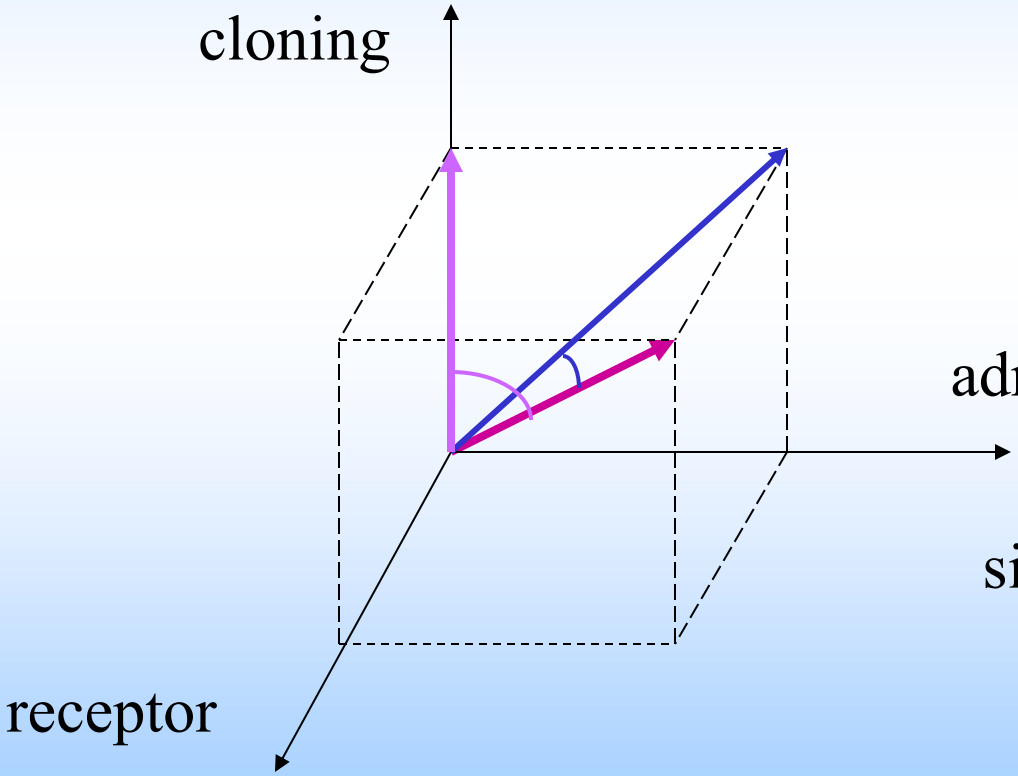
  boolesk, vektor, probabilistisk, …
- filmodell:

  flat fil, inverterad fil, ...

IR - Filmodell: inverterad fil



Vektormodellen (förenklad)



Doc1 (1,1,0)

Doc2 (0,1,0)

Q (1,1,1)

$$sim(d,q) = \frac{d \cdot q}{|d| \times |q|}$$

Databaser

- Relationsdatabaser:
  - modell: tabeller + relationsalgebran
  - frågespråk (SQL)
- Objektorienterade databaser:
  - modell: fortlevande objekt, meddelande, inkapsling, ärvning
  - frågespråk (t.ex. OQL)
- System: GDB (R), ACEDB (OO)

Relationsdatabaser

PROTEIN

PROTEIN-ID	ACCESSION	DEFINITION	SOURCE
1	NM_000684	Homo sapiens adrenergic, beta-1-, receptor	human

REFERENCE

PROTEIN-ID	ARTICLE-ID
1	1
1	2

ARTICLE

ARTICLE-ID	AUTHOR	TITLE
1	Frielle	Cloning of the cDNA for the human ….
1	Collins	Cloning of the cDNA for the human ….
1	Daniel	Cloning of the cDNA for the human ….
1	Caron	Cloning of the cDNA for the human ….
1	Lefkowitz	Cloning of the cDNA for the human ….
1	Kobilka	Cloning of the cDNA for the human ….
2	Frielle	Human beta 1- and beta 2-adrenergic receptors
2	Kobilka	Human beta 1- and beta 2-adrenergic receptors
2	Lefkowitz	Human beta 1- and beta 2-adrenergic receptors
2	Caron	Human beta 1- and beta 2-adrenergic receptors

Relationsdatabaser

PROTEIN

PROTEIN-ID	ACCESSION	DEFINITION	SOURCE
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REFERENCE

PROTEIN-ID	ARTICLE-ID
1	1
1	2

ARTICLE-AUTHOR

ARTICLE-ID	AUTHOR
1	Frielle
1	Collins
1	Daniel
1	Caron
1	Lefkowitz
1	Kobilka
2	Frielle
2	Kobilka
2	Lefkowitz
2	Caron

ARTICLE-TITLE

ARTICLE-ID	TITLE
1	Cloning of the cDNA for the human beta 1-adrenergic receptor
2	Human beta 1- and beta 2-adrenergic receptors: structurally and functionally related receptors derived from distinct genes

SQL

select source
from protein
where accession = NM_000684;

Vilka kolumner?
Vilka tabeller?
Vilka rader?

PROTEIN

PROTEIN-ID	ACCESSION	DEFINITION	SOURCE
1	NM_000684	Homo sapiens adrenergic, beta-1-, receptor	human

SQL

```
select title
from protein, article-title, reference
where protein.accession = NM_000684
  and protein.protein-id
                = reference.protein-id
  and reference.article-id
                = article-title.article-id;
```

REFERENCE

PROTEIN-ID	ARTICLE-ID
1	1
1	2

PROTEIN

PROTEIN-ID	ACCESSION	DEFINITION	SOURCE
1	NM_000684	Homo sapiens adrenergic, beta-1-, receptor	human

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ARTICLE-ID	TITLE
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2	Human beta 1- …

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select title
from protein, article-title, reference
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                = reference.protein-id
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```

REFERENCE

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                = article-title.article-id;
```

REFERENCE

PROTEIN-ID	ARTICLE-ID
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1	1
1	2

SQL

```
select title
from protein, article-title, reference
where protein.accession = NM_000684
  and protein.protein-id
                = reference.protein-id
  and reference.article-id
                = article-title.article-id;
```

REFERENCE

PROTEIN-ID	ARTICLE-ID
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1	2

PROTEIN

PROTEIN-ID	ACCESSION	DEFINITION	SOURCE
1	NM_000684	Homo sapiens adrenergic, beta-1-, receptor	human

ARTICLE-TITLE

ARTICLE-ID	TITLE
1	Cloning of the …
2	Human beta 1- …

					REFERENCE	ARTICLE-TITLE	
PROTEIN-ID	ACCESSION	DEFINITION	SOURCE	PROTEIN-ID	ARTICLE-ID	ARTICLE-ID	TITLE
1	NM_000684	Homo sapiens adrenergic, beta-1-, receptor	human	1	1	1	Cloning of the …
1	NM_000684	Homo sapiens adrenergic, beta-1-, receptor	human	1	2	2	Human beta 1- …

SQL

```
select title
from protein, article-title, reference
where protein.accession = NM_000684
  and protein.protein-id
                = reference.protein-id
  and reference.article-id
                = article-title.article-id;
```

REFERENCE

PROTEIN-ID	ARTICLE-ID
1	1
1	2

PROTEIN

PROTEIN-ID	ACCESSION	DEFINITION	SOURCE
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ARTICLE-TITLE

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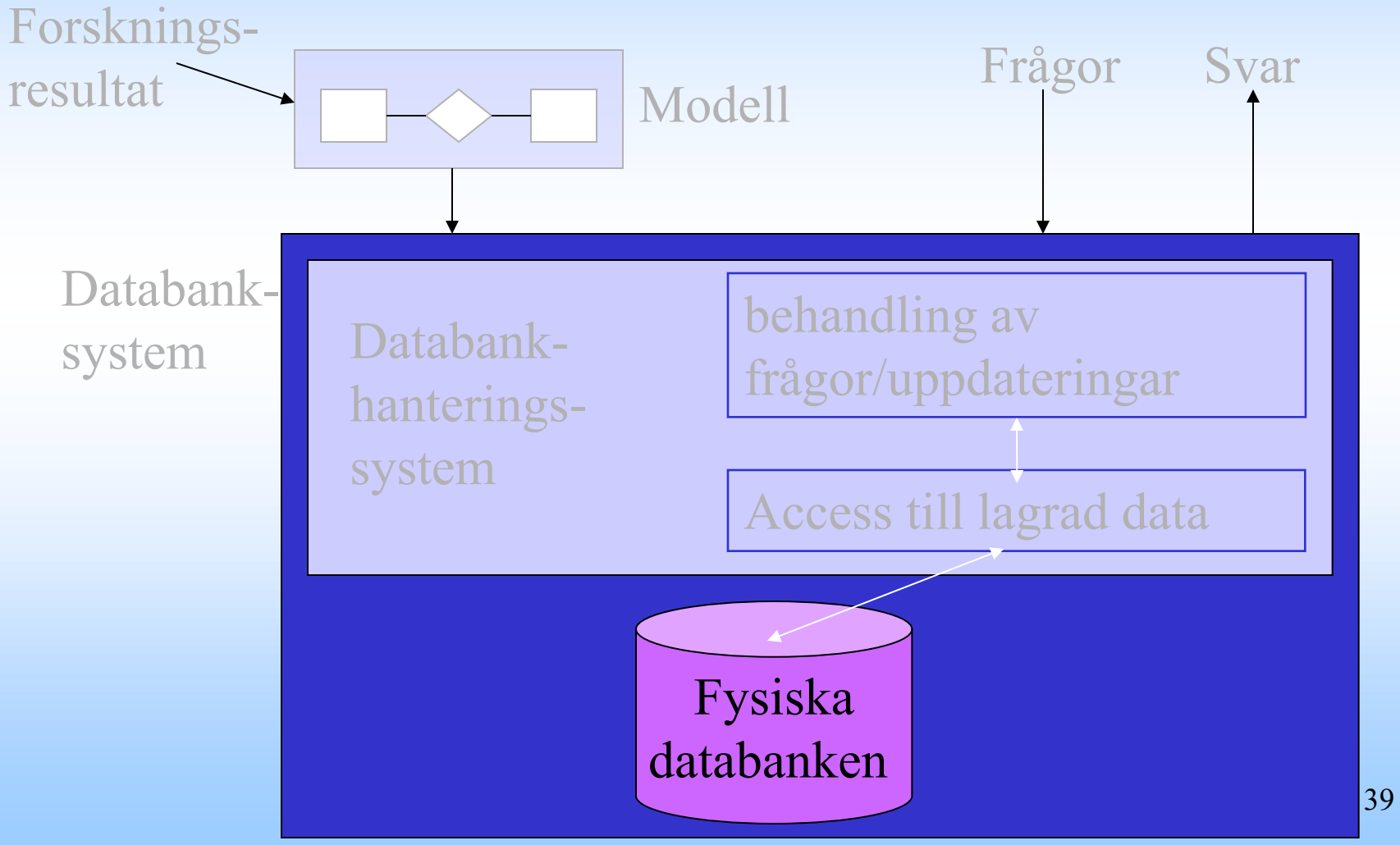
1	NM_000684	Homo sapiens adrenergic, beta-1-, receptor	human	1	1	1	Cloning of the …
1	NM_000684	Homo sapiens adrenergic, beta-1-, receptor	human	1	2	2	Human beta 1- …

TITLE

Cloning of the …

Human beta 1- …

Hur lagras informationen? (låg nivå)



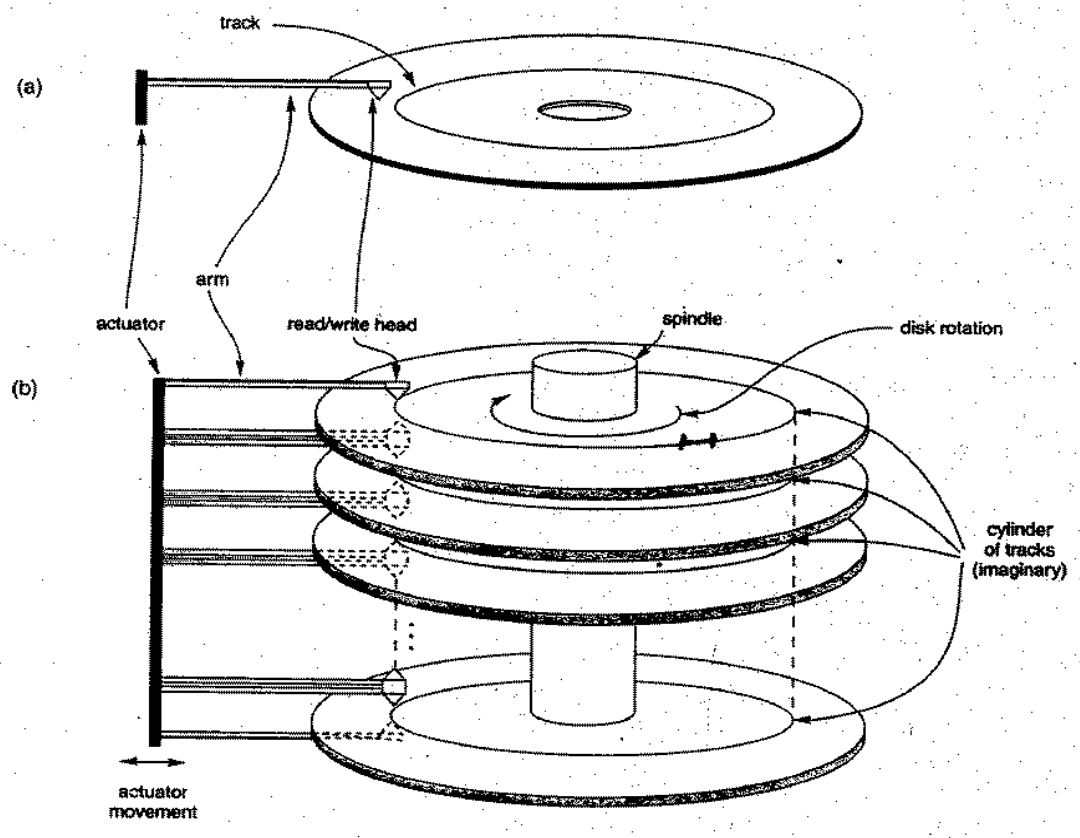
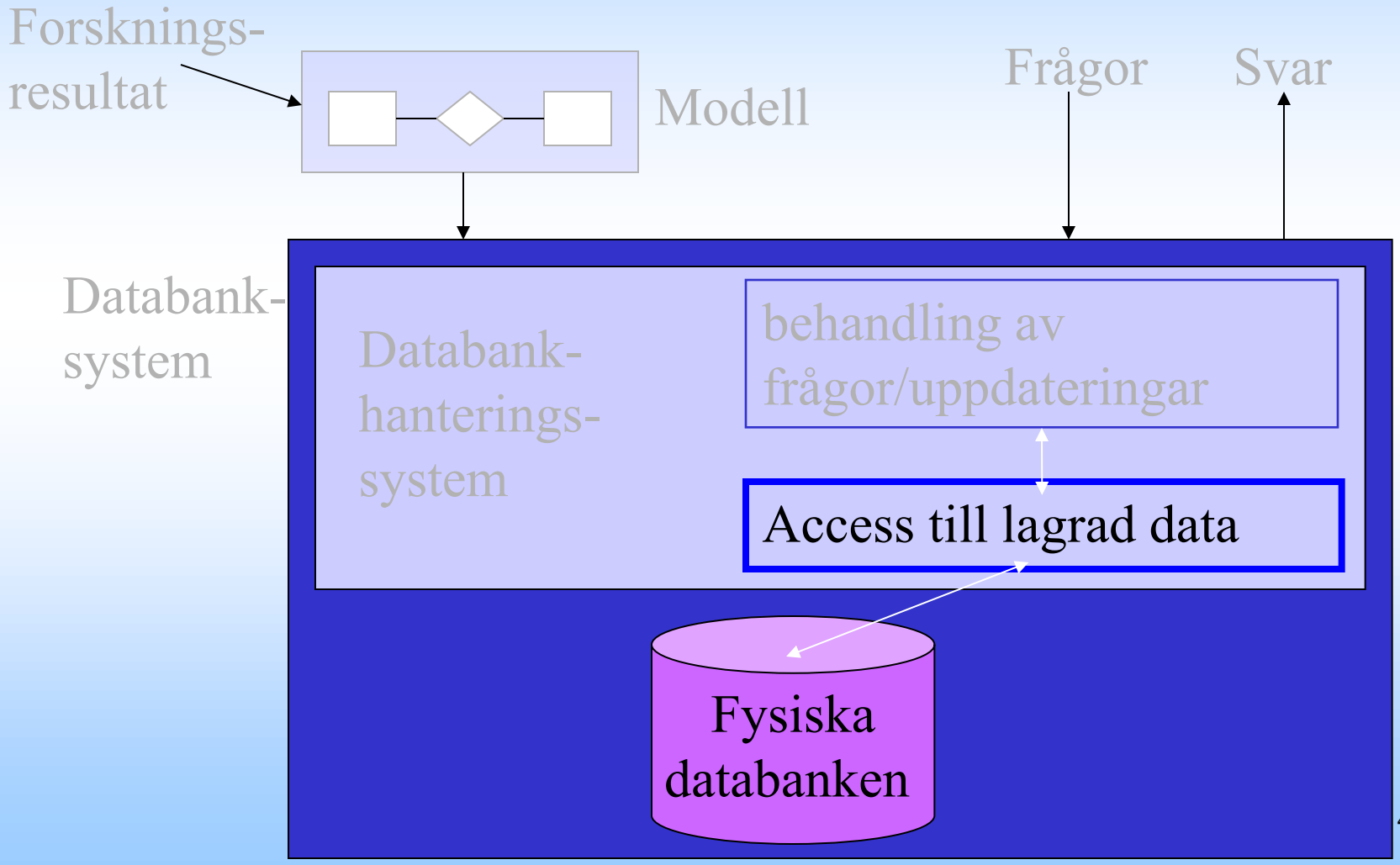


Figure 5.1 (a) A single-sided disk with read/write hardware. (b) A disk pack with read/write hardware.

Hur accessar man informationen? (systemnivå)

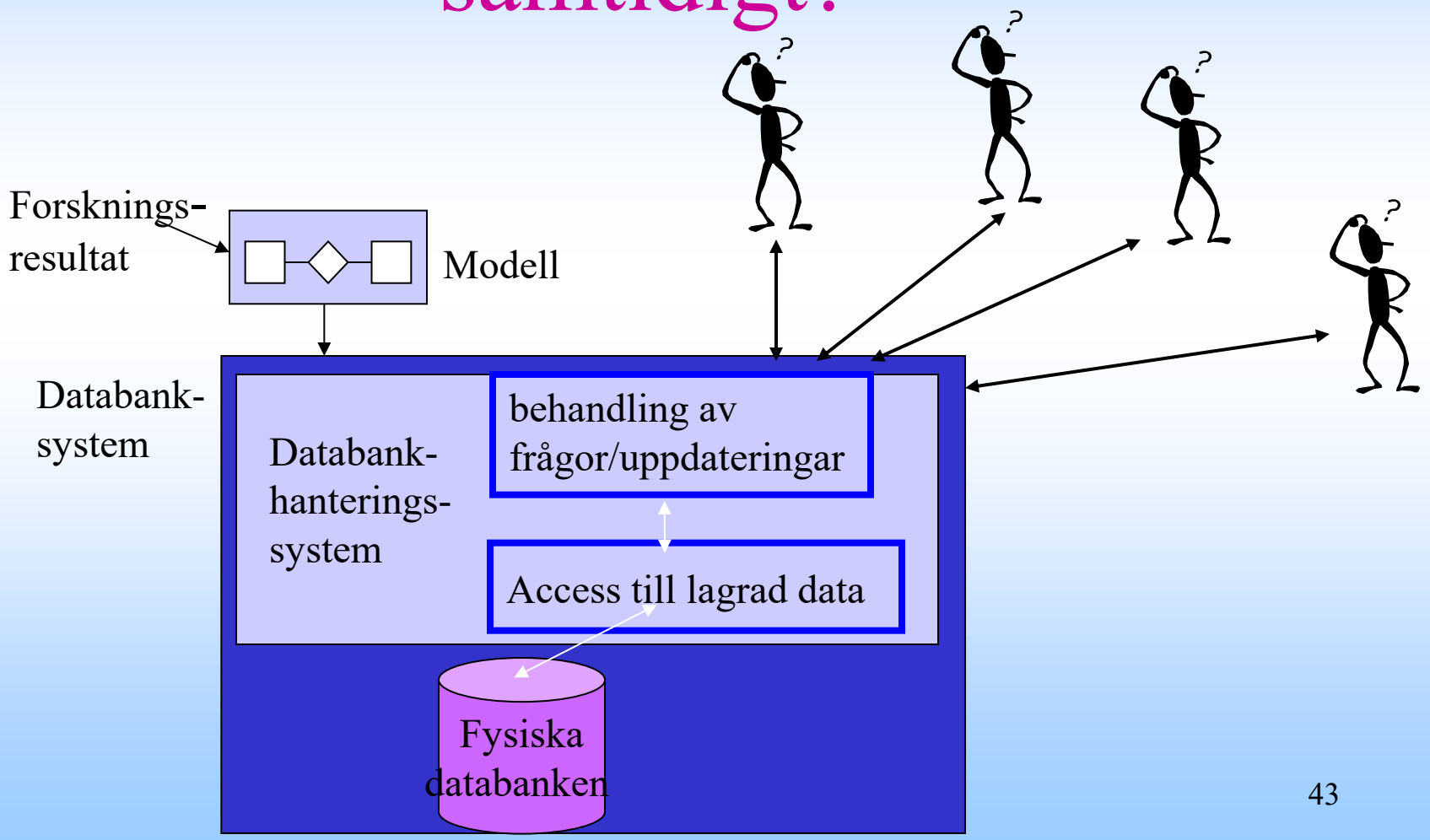


Hur återställer man en databank efter crash?

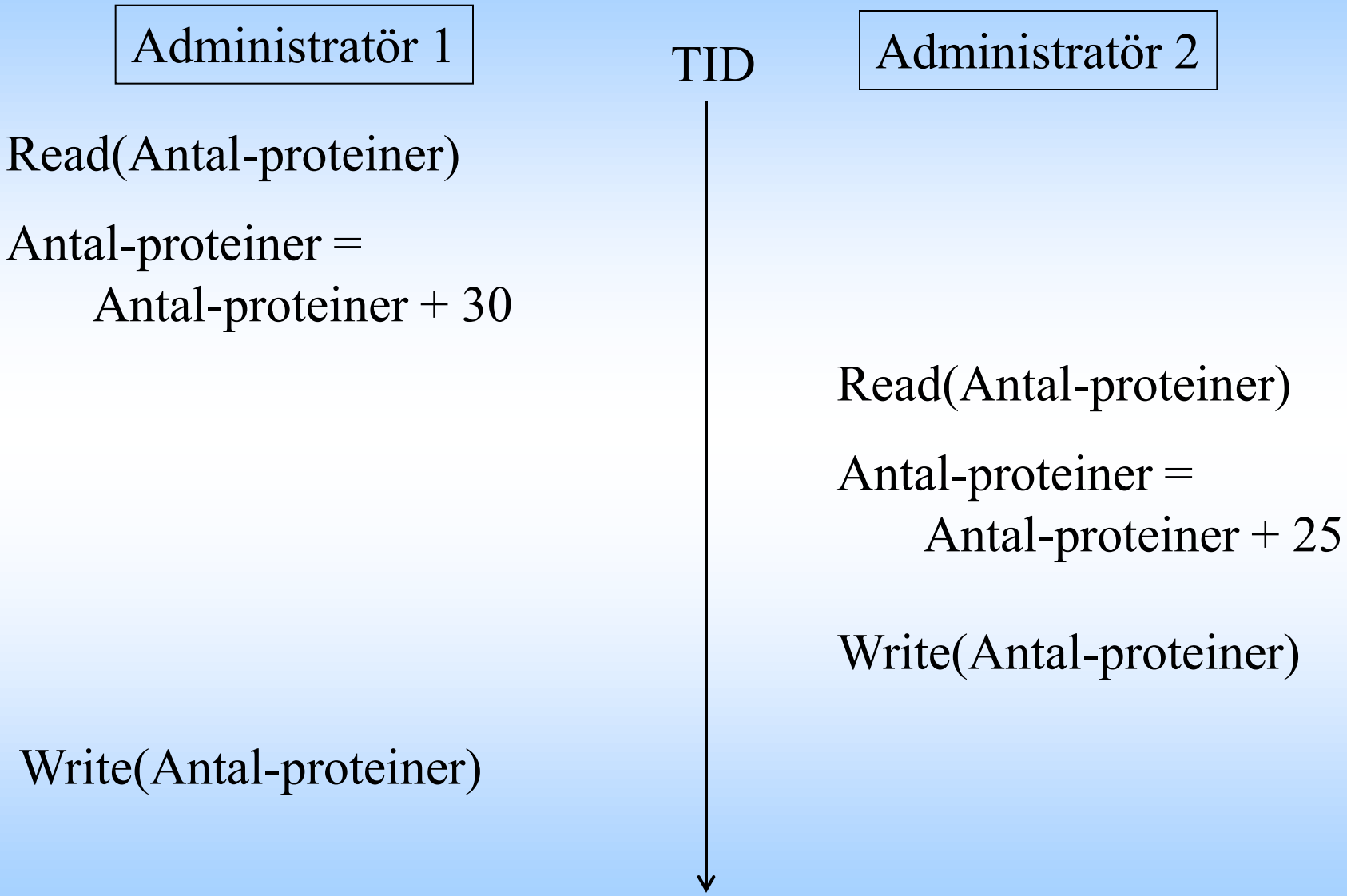
Återställning vid

- datorstop (system crash)
- systemfel
- samtidighetsfel (flera användare)
- skivfel
- katastrofer

Hur kan flera användare accessa och uppdatera informationen samtidigt?

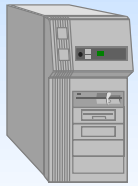


Flera användare



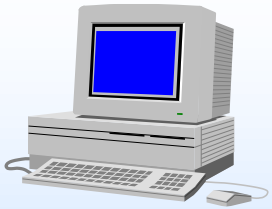
Flera användare

DB

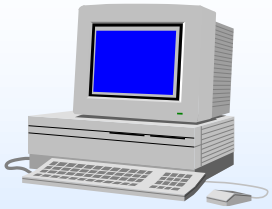


Antal-proteiner: 150

A1



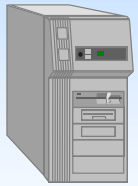
A2



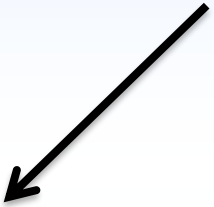
Flera användare

DB

A1: Read(Antal-proteiner)

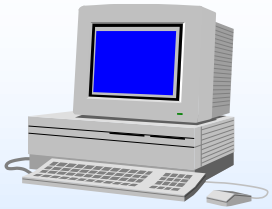


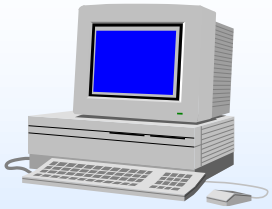
Antal-proteiner: 150



A1

A2



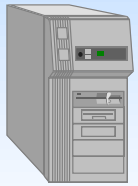


Antal-proteiner: 150

Flera användare

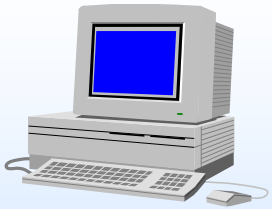
DB

A1: Antal-proteiner =
Antal-proteiner + 30

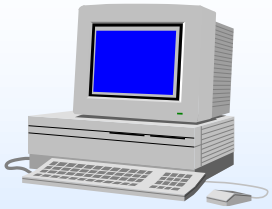


Antal-proteiner: 150

A1



A2

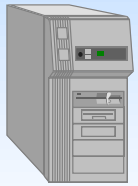


Antal-proteiner: 150 + 30

Flera användare

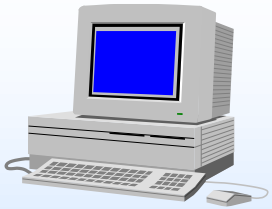
DB

A1: Antal-proteiner =
Antal-proteiner + 30

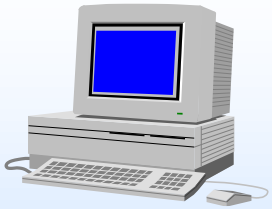


Antal-proteiner: 150

A1



A2

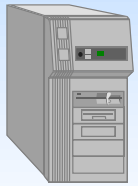


Antal-proteiner: 180

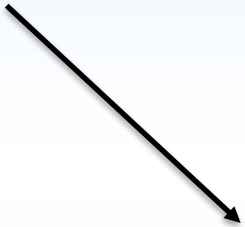
Flera användare

DB

A2: Read(Antal-proteiner)

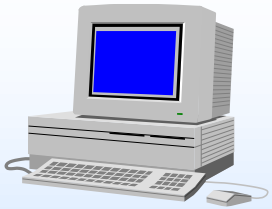


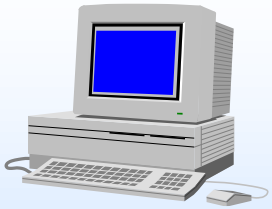
Antal-proteiner: 150



A1

A2





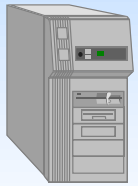
Antal-proteiner: 180

Antal-proteiner: 150

Flera användare

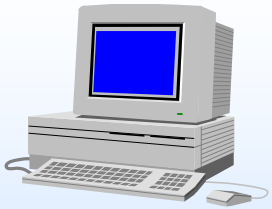
DB

A2: Antal-proteiner =
Antal-proteiner + 25

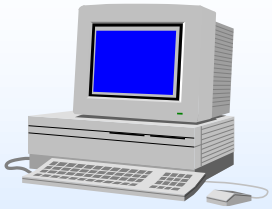


Antal-proteiner: 150

A1



A2



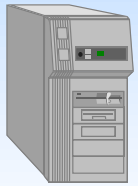
Antal-proteiner: 180

Antal-proteiner: 150 +25

Flera användare

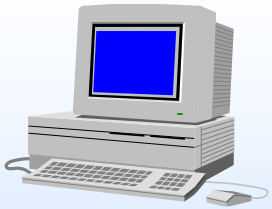
DB

A2: Antal-proteiner =
Antal-proteiner + 25

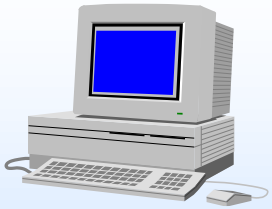


Antal-proteiner: 150

A1



A2



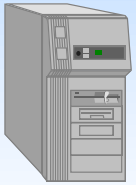
Antal-proteiner: 180

Antal-proteiner: 175

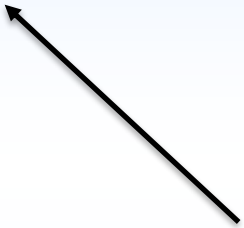
Flera användare

DB

A2: Write(Antal-proteiner)

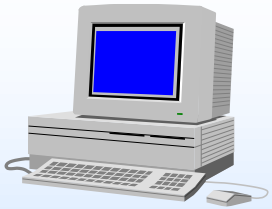


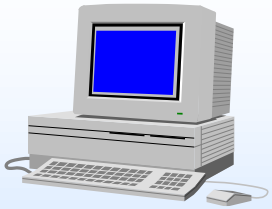
Antal-proteiner: ~~150~~



A1

A2





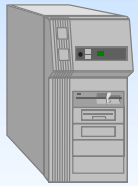
Antal-proteiner: 180

Antal-proteiner: 175

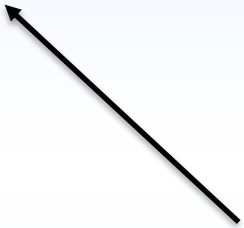
Flera användare

DB

A2: Write(Antal-proteiner)

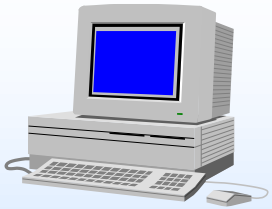


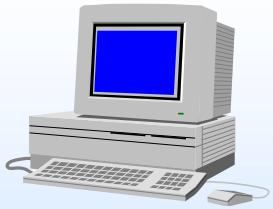
Antal-proteiner: 175



A1

A2





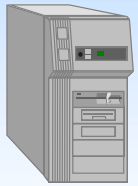
Antal-proteiner: 180

Antal-proteiner: 175

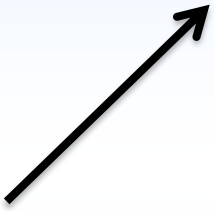
Flera användare

DB

A1: Write(Antal-proteiner)

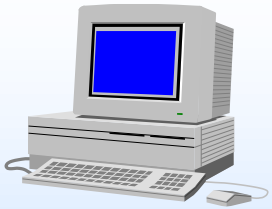


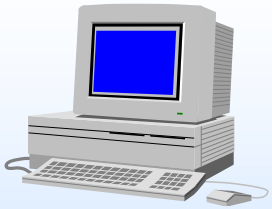
Antal-proteiner: ~~175~~



A1

A2





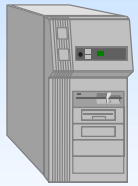
Antal-proteiner: 180

Antal-proteiner: 175

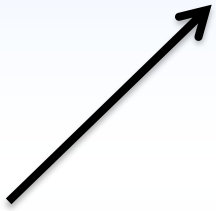
Flera användare

DB

A1: Write(Antal-proteiner)

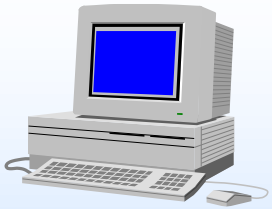


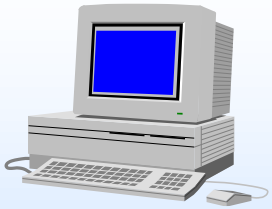
Antal-proteiner: 180



A1

A2



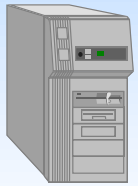


Antal-proteiner: 180

Antal-proteiner: 175

Flera användare

DB



Antal-proteiner: 180

Antal-proteiner: 150 + 30 + 25 = 205

Informationssäkerhet

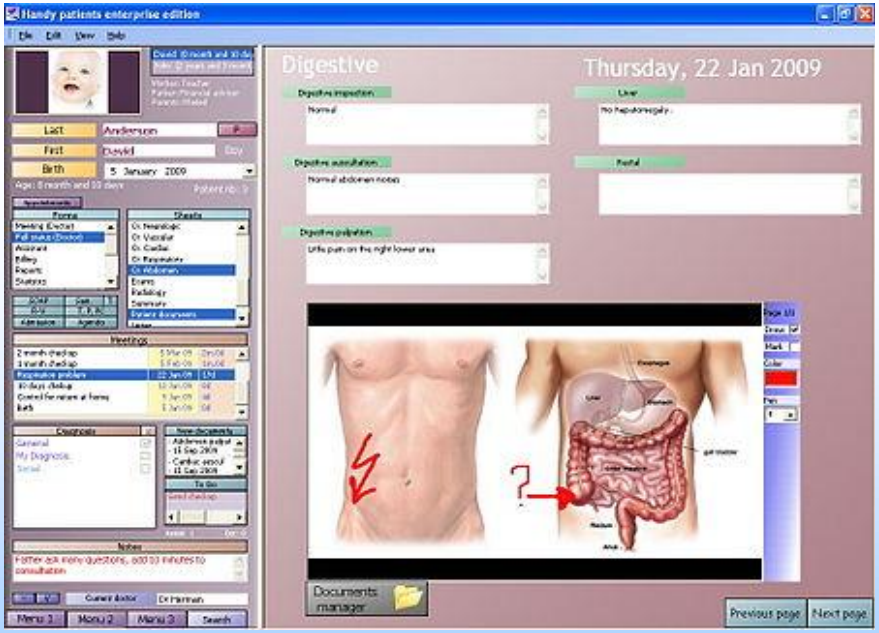
Sekretess

Enbart behöriga användare får ta del av informationen

Integritet

Korrekt och fullständig information

Tillgänglighet



https://en.wikipedia.org/wiki/Electronic_health_record

Kursöversikt - FÖ

- Introduktion
- Relationsdatabaser och SQL
- Datamodellering, ER/EER diagram
- Att gå från EER diagram till relationsscheman

Kursöversikt - FÖ

- Informationssäkerhet
- Databassäkerhet

Kursöversikt - LA+projekt

- Lab1: Grundläggande SQL
- Lab2: Databasdesign och EER modellering
- Lab3: Avancerad SQL
- Lab4: Informationssäkerhet

Kursöversikt - LA+projekt

- ’Lab5’: Projekt i bioinformatik

  genomdatabas

  proteindatabas

  enzymdatabas

  databas för biologiska reglersystem

Kursöversikt - LA+projekt

- Rapporteringsdeadline vid varje tentamenstillfälle
- behövs ett särskilt databaskonto

--> automatisk vid registrering på kursen

databaskontona tas bort efter 1 år

- anmälan till laborationer via kurshemsidan **senast 9 september**

Examination

- tenta
- laborationsserie
- projekt

En kurs för TB

- Användning i senare kurser + arbete
- Unik och eftertraktad kompetens
  - Bio
  - Data
  - Förståelse av modellering + konsekvenser (Hur modellera? Hur ställa frågor? Värför går det långsamt? Varför får man inget svar?...)