A Formal Analysis of Algorithms for Matroids and Greedoids

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December 2, 2025

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Technische Universität München, Germany

Abstract

We present a formal analysis, in Isabelle/HOL [30], of optimisation algorithms for matroids, which are useful generalisations of combinatorial structures that occur in optimisation, and greedoids, which are a generalisation of matroids. Although some formalisation work has been done earlier on matroids, our work here presents the first formalisation of results on greedoids, and many results we formalise in relation to matroids are also formalised for the first time in this work. We formalise the analysis of a number of optimisation algorithms for matroids and greedoids. We also derive

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Background

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- combinatorial optimisation: optimisation problems on discrete structures, e.g. graphs

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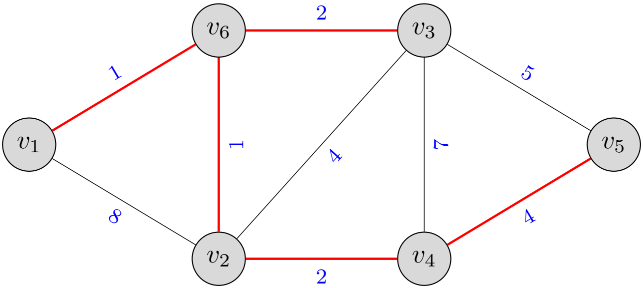

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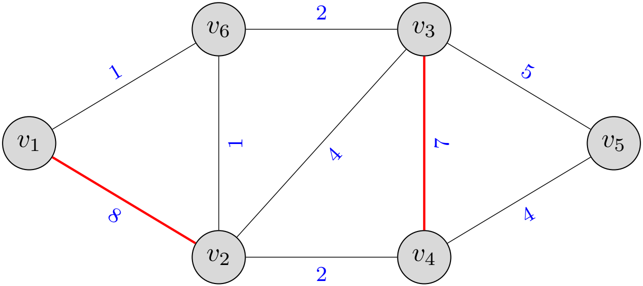

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```
fun fac :: nat ⇒ nat where
  fac 0 = 1 |
  fac n = n * fac (n -1)

lemma log-fac-bounds:
  ∃ (c1 :: real) (c1 :: real).
    c1*n*ln n  ≤ ln (fac n)  ≤ c2*n*ln n
       ∧  c1 > 0  ∧  c2 > 0
```

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- both theoretical and practical interest

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Definition (Independence System)

A *ground set* E and a family of *independent sets* $\mathcal{F} \subseteq \mathcal{P}(E)$ is an independence system $(E, \mathcal{F})$ iff

M1. $\emptyset \in \mathcal{F}$

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Definition (Basis)

A basis B of $A \subseteq E$ is an inclusion-maximal independent subset of A. A basis of the independence system $\mathcal{F} \subseteq \mathcal{P}(E)$ is a basis of E.

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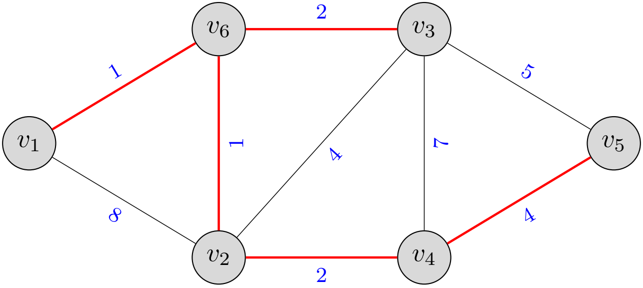

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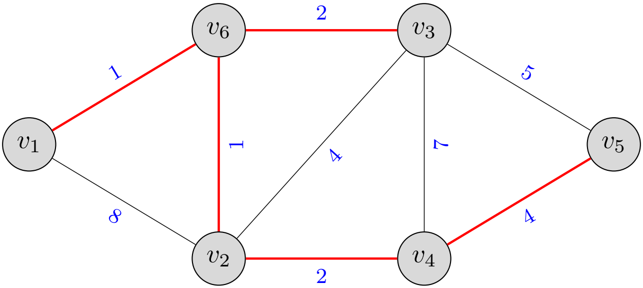

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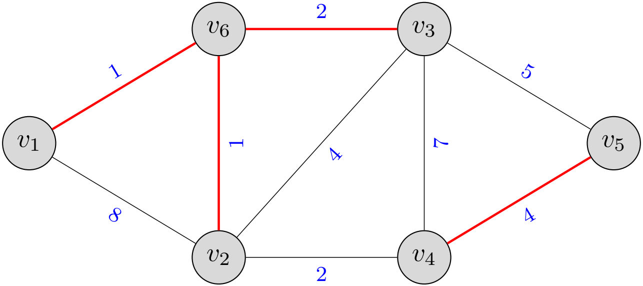

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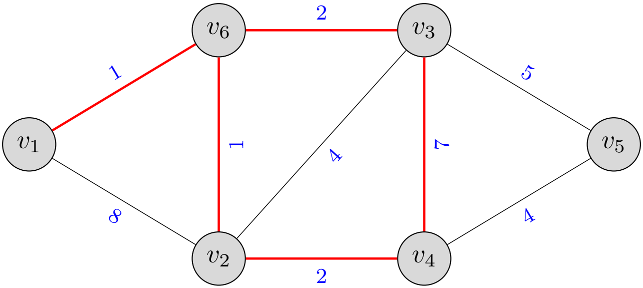

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- independent sets are forests
- bases are spanning trees
- maximum weight forest is maximum weight independent set
- minimum spanning tree is minimum weight basis

Theory of Matroids and Greedoids (Selection)

- Whitney (1935): introduction of matroids
- Tutte (1965): Lectures on Matroids, Homotopy Theorem
- Edmonds (1970, 1971): greedy algorithms, Matroid Intersection Theorem
- Lawler (1975): matroid intersection algorithms
- Seymour (1980): Decomposition Theorem for Regular Matroids
- Korte and Lovasz (1980): greedoids and greedy algorithms
- many concepts: set system, independence system, matroid, basis, circuit, rank, rank quotient, closure operator, greedoid, accessibility, etc. etc.

our main reference:

- *Combinatorial Optimization (6th Edition)* by Korte and Vygen

Formalisation of Matroids

- Mizar: basic matroid theory [Bancerek and Shidama 2008]
- Coq/Rocq: projective geometry and Desargues theorem [Magaud et al. 2012]
- Isabelle/HOL: basic matroid theory [Keinholz 2018], basis for our work
- Isabelle/HOL: Kruskal's Algorithm [Haslbeck et al. 2018], most related
- Lean: matroid theory [Nelson et al. github, 2023 - ongoing]
- Coq/Rocq: matroid-based automated prover [Magaud et al. 2024]

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Algorithm 1: BestInGreedy$(E, \mathcal{F}, c)$

[Rado 1957, Edmonds 1971, Jenkyns 1976, Korte and Hausmann 1978]

Sort $E := \{e_1, \ldots, e_n\}$ such that $c(e_1) \geq c(e_2) \geq \ldots \geq c(e_n)$;
$F \leftarrow \emptyset$;
for $i := 1$ *to* n **do**
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- concrete problem: focus on implementing oracle

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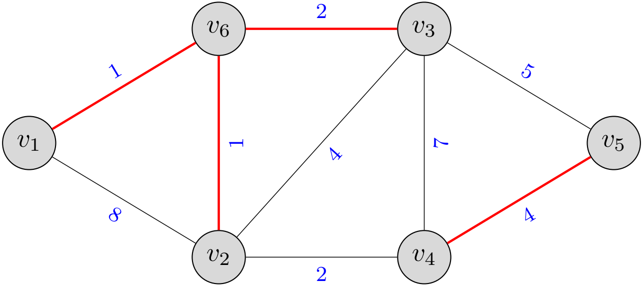
- red edges are acyclic, i.e. independent
- adding blue edge preserves independence



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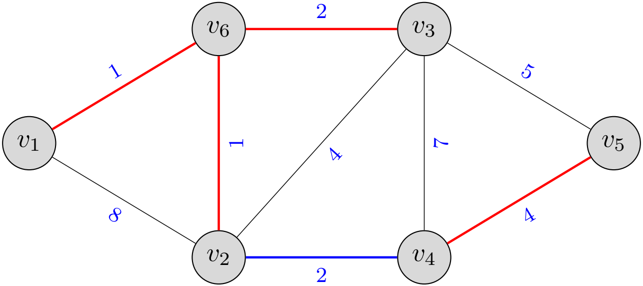

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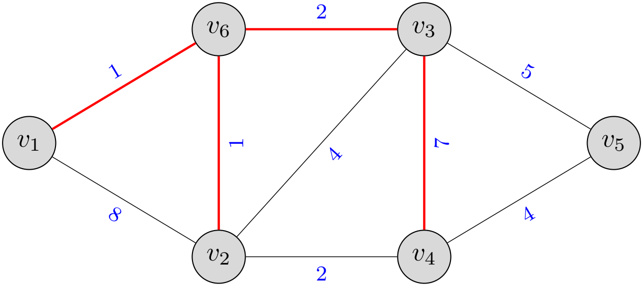

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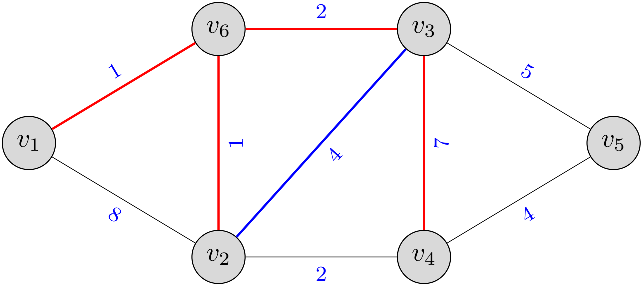

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- given $T \subseteq E$ acyclic, $e \in E \setminus T$, is $T \cup \{e\}$ still acyclic?
- yes, iff endpoints x and y of e in different connected components of T
- is there path in T between x and y?
- Depth-First Search (our approach) or Breadth-First Search
- Union-Find for components of T (Haslbeck et al. with Imperative HOL and Refinement Framework)
- this is Kruskal's Algorithm

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- *independence oracle:* if $e \in E \setminus F$ and $F \in \mathcal{F}$, is $F \cup \{e\} \in \mathcal{F}$?

Formalisation of Algorithm

```
locale Best-In-Greedy = matroid: Matroid-Specs
  where set-empty = set-empty for set-empty :: 'set +
  fixes carrier :: 'set and indep :: 'set ⇒ bool
    and sort-desc :: ('set ⇒ rat) ⇒ 'a list ⇒ 'a list
    and indep-oracle::'a ⇒ 'set ⇒ bool
```

Formalisation (Loop)

```
function BestInGreedy ::
    ('a, 'set) best-in-greedy-state
     ⇒ ('a, 'set) best-in-greedy-state
where
BestInGreedy state  =
 (case (carrier-list state) of
  [] ⇒ state |
  (x # xs) ⇒
  (if  indep-oracle  x (result state) then
      let new-result = (set-insert x (result state)) in
          BestInGreedy
           (state ⦇carrier-list :=  xs, result :=  new-result⦈)
   else  BestInGreedy  (state ⦇carrier-list :=  xs⦈)))

definition initial-state c order =
  ⦇carrier-list = (sort-desc c order), result = set-empty⦈
```

Formalisation (Independence Oracle, simplified)

- if $e \in E \setminus F$ and $F \in \mathcal{F}$, is $F \cup \{e\} \in \mathcal{F}$?

```
context
 assumes local-indep-oracle:
  ⋀   F :: 'set  e :: 'a.
    ⟦ set-inv F; indep F; subseteq F carrier; e ∉ to-set F ⟧
    ⟹  indep-oracle e F  ⟷  indep (set-insert e F)
 and carrier-inv: set-inv carrier
```

Executability

- data structures to implement sets
- operations and behaviour specified by locale

```
locale Set =
fixes empty :: 's
fixes insert :: 'a ⇒ 's ⇒ 's
fixes delete :: 'a ⇒ 's ⇒ 's
...
fixes set :: 's ⇒ 'a set
fixes invar :: 's ⇒ bool
assumes set-empty:    set empty = {}
assumes set-insert:   invar s
                 ⟹  set(insert x s) = set s ∪ {x}
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- abstract data types
  [Wirth 1971, Hoare 1972, Liskov and Zilles 1974]

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- instantiation to obtain executable algorithms for concrete problems, e.g. Kruskal's Algorithm (for MWF)
- generic for different implementations and matroids
- stepwise refinement [Wirth 1971 + Hoare 1972]:
  replace instruction (e.g. $F \cup \{e\} \in \mathcal{F}$?) with more detailed instructions (e.g. does e add a cycle to F?)

Formalisation of the Oracle for Kruskal

```
definition local-indep-oracle e X =
((Card-Set2-RBT.subseteq (vset-insert e X) input-G)  ∧
 (lookup (Kruskal-E-to-G X) (fst e)  ≠  None
   ∧  lookup (Kruskal-E-to-G X) (snd e)  ≠  None ⟶
      return (dfs-impl (Kruskal-E-to-G X) (snd e)
        (dfs-initial-state (fst e))) = NotReachable))
```

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- preserved by loop iterations
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- preserved by loop iterations
- induction over loop execution

At the beginning of the loop body

- $F \subseteq E$
- $F \in \mathcal{F}$
- current `carrier-list` is $[e_i, ..., e_n]$ for current iteration i.
  (NB: $i = |E| - |$`carrier-list`$|$)
- current `result` is subset of $\{e_1, ..., e_{i-1}\}$
- $\forall 0 \leq j \leq i-1$:
  $\texttt{result}_j (= \{e_1, ..., e_{j-1}\} \cap \texttt{result})$ is basis of $\{e_1, ..., e_{j-1}\}$.

Properties of the Algorithm

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Theorem (Cost Bound [Jenkyns 1976, Korte and Hausmann 1978])
Let $(E, \mathcal{F})$ be an independence system, with $c : E \to \mathbb{R}_+$. Let F be the output of BestInGreedy. Then $c(F) \geq q(E, \mathcal{F}) \cdot \max_{X \in \mathcal{F}} c(X)$.

- $q(E, \mathcal{F})$ is the *rank quotient*, a number associated with every independence system
- $q(E, \mathcal{F}) = 1$ iff $(E, \mathcal{F})$ is matroid

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- different proof for Corollary 2 already formalised by Haslbeck, Lammich and Biendarra (2018, see AFP).

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Theorem (Tightness [Jenkyns 1976, Korte and Hausmann 1978])

Let $(E, \mathcal{F})$ be an independence system. There exists a cost function $c : E \to \mathbb{R}_+$ s.t. for the output F of BestInGreedy*,*
$c(F) = q(E, \mathcal{F}) \cdot \max_{X \in \mathcal{F}} c(X)$.

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Theorem (Characterisation [Rado 1957, Edmonds 1971])

An independence system $(E, \mathcal{F})$ is a matroid if and only if BestInGreedy *finds an optimal solution for the maximum weight independent set problem for $(E, \mathcal{F}, c)$ for all cost functions $c : E \to \mathbb{R}_+$.*

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Greedoids

Greedoids

Definition (Greedoid)

A *ground set* E and a family of *independent sets* $\mathcal{F} \subseteq \mathcal{P}(E)$ is a greedoid iff

M1. $\emptyset \in \mathcal{F}$

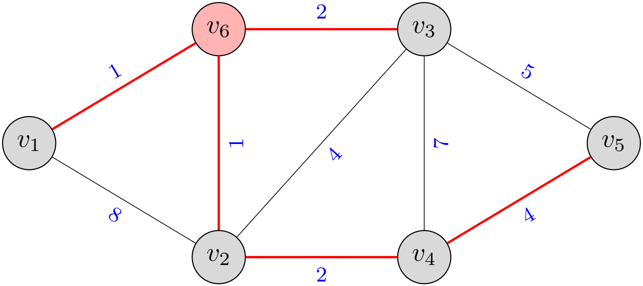
M3. $A \in \mathcal{F}$ and $B \in \mathcal{F}$ and $|B| > |A|$
then $\exists x \in B \setminus A.\ A \cup \{x\} \in \mathcal{F}$

Formalisation

```
locale greedoid =
  fixes E :: 'a set
  fixes F :: 'a set set
  assumes contains-empty-set: {} ∈ F
  and finite-E: finite E
  and in-F-in-E: ⋀ X. X ∈ F ⟹ X ⊆ E
  and third-condition:
     ⋀ X Y. ⟦ (X ∈ F);(Y ∈ F) ; (card X > card Y) ⟧
     ⟹ ∃x ∈ X - Y. Y ∪ {x} ∈ F
```

Greedoids: An Example

- for a vertex r, $T \subseteq E$ is an *arborescence* around r iff
  - T is a tree
  - r is in T
- for fixed r, set of arborescences satisifies M1+M3



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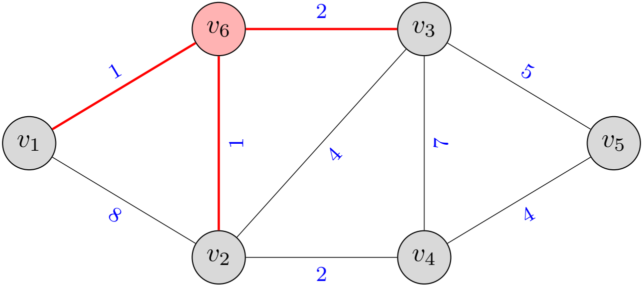

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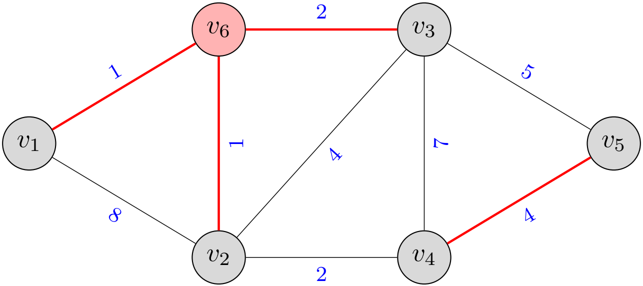

Properties of Greedoids

- greedoids are *accessible*
- *antimatroids* are greedoids
- *closure* operators
- *anti-exchange* property
- *strong exchange* property
- an algorithm ...

Greedoid Algorithm

Algorithm 2: GreedoidGreedy$(E, \mathcal{F}, c)$

$F \leftarrow \emptyset$;
while $\exists e \in E \setminus F.\ F \cup \{e\} \in \mathcal{F}$ **do**
  find $e \in E \setminus F$ with $F \cup \{e\} \in \mathcal{F}$ where $c(F \cup \{e\})$ is maximum;
  $F \leftarrow F \cup \{e\}$;
return F;

- as long as $\exists$ element to extend F, add the element e maximising $c(F \cup \{e\})$.
- independence oracle: if $e \in E \setminus F$ and $F \in \mathcal{F}$, is $F \cup \{e\} \in \mathcal{F}$?

Formalisation

```
definition find-best-candidate es c F' =  foldr (λ e acc.
  if e ∈ F' ∨ ¬ (orcl e F') then acc
  else (case acc of None ⇒ Some e |
                    Some d ⇒
    (if elements-costs c e > elements-costs c d then Some e
     else Some d))) es None

function (domintros) greedoid-greedy ::
  'a list ⇒ ('a set ⇒ real) ⇒ 'a list ⇒ 'a list  where
  greedoid-greedy es c  xs =
 (case  (find-best-candidate es c  (set xs)) of
      Some e ⇒ greedoid-greedy es c  (e#xs)
    | None ⇒ xs)
```

Properties of Greedoid Algorithm

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Properties of Greedoid Algorithm

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Theorem (Korte and Vygen: Characterisation of Strong-Exchange Greedoids)

We fix a greedoid $(E, \mathcal{F})$*.* GreedoidGreedy *computes a maximum-weight basis in* $\mathcal{F}$ *for any order of iteration* $e_1, ..., e_n$ *and any modular cost function* $c : \mathcal{P}(E) \to \mathbb{R}$ *iff* $(E, \mathcal{F})$ *has the strong exchange property (SEP).*

- modular weight function: $c(A \cup B) = c(a) + c(B) - c(A \cap B)$ for all $A, B \subseteq E$
- SEP: for all A, $B \in \mathcal{F}$, B basis w.r.t $\mathcal{F}$, $A \subseteq B$ and $x \in E \setminus B$ with $A \cup \{x\} \in \mathcal{F}$, there is y with $A \cup \{y\} \in \mathcal{F}$ and $(B - \{y\}) \cup \{x\} \in \mathcal{F}$.

```
theorem greedoid-characterisation:
(∀ c es. valid-modular-weight-func E c  ∧   E = set es
         ∧  distinct es
         ⟶ opt-basis c (set (greedoid-greedy es c Nil)))
 ⟷  strong-exchange-property E F
```

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Matroid Intersection

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- two matroids $(E, \mathcal{F}_1)$ and $(E, \mathcal{F}_2)$

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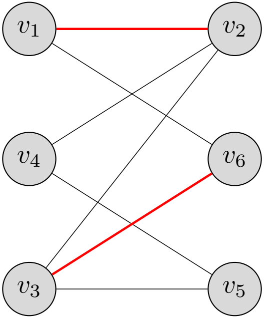
- example: maximum cardinality bipartite matching

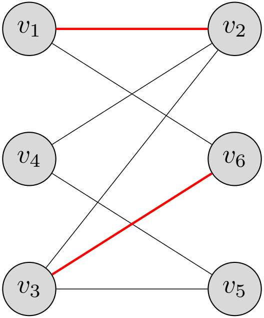
Matroid Intersection: Example

- matching: set of vertex disjoint edges
- bipartite: edges only between left and right



Matroid Intersection: Example

- two matroids $(E, \mathcal{F}_L)$ and $(E, \mathcal{F}_R)$
- $F \in \mathcal{F}_L$ iff no $e,\ f \in F$ share left endpoint
- $F \in \mathcal{F}_R$ iff no $e,\ f \in F$ share right endpoint



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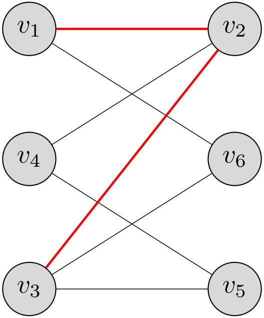

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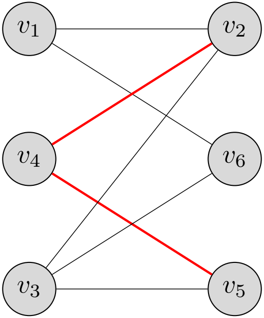

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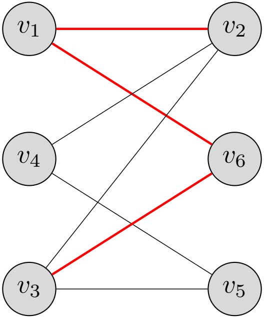

Theorem (Rank Criterion, Edmonds' Intersection Theorem)

For two matroids $(E, \mathcal{F}_1)$ *and* $(E, \mathcal{F}_2)$ *with rank functions* r_1 *and* r_2*, respectively,* $X \in \mathcal{F}_1 \cap \mathcal{F}_2$*, and* $Q \subseteq E$ *it holds that* $|X| \leq r_1(Q) + r_2(E \setminus Q)$*. Therefore,* $|X| \leq r_1(X) + r_2(E \setminus X)$*, for any* $X \in \mathcal{F}_1 \cap \mathcal{F}_2$*.*

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Intersection Algorithm: Idea

- M2: $A \in \mathcal{F}$ and $B \subseteq A \implies B \in \mathcal{F}$
- M3: $A \in \mathcal{F}$ and $B \in \mathcal{F}$ and $|B| > |A|$
  $\implies \exists x \in B \setminus A.\ A \cup \{x\} \in \mathcal{F}$
- assume $F \in \mathcal{F}_1 \cap \mathcal{F}_2$ with $|F| < |F'|$ where $F' \in \mathcal{F}_1 \cap \mathcal{F}_2$
- by M3: find e_0 with $F \cup \{e_0\} \in \mathcal{F}_1$
- if $F \cup \{e_0\} \in \mathcal{F}_2$, add e_0 to F

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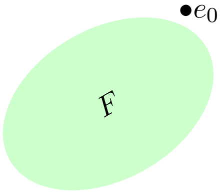

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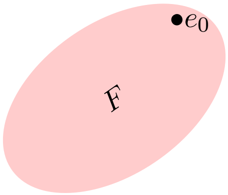
- add e_0 to F, breaks independence w.r.t. $\mathcal{F}_2$



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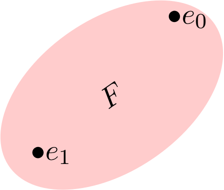
- remove some e_1 from F



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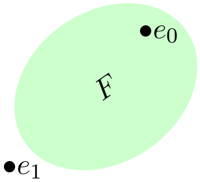
- $F \cup \{e_0\} \in \mathcal{F}_1$ but $F \cup \{e_0\} \notin \mathcal{F}_2$
- remove some e_1 from $F \Rightarrow$ independence w.r.t. $\mathcal{F}_2$



- set $F = F \cup \{e_0\} \setminus \{e_1\}$

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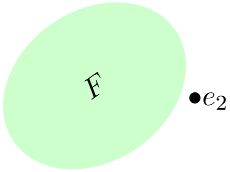

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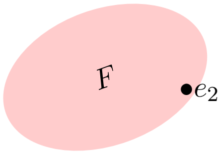

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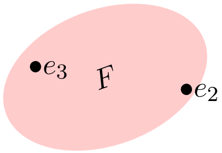

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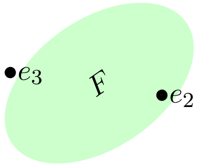
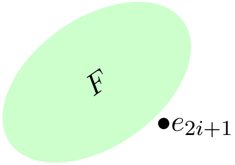


- set $F = F \cup \{e_2\} \setminus \{e_3\}$

Intersection Algorithm: Idea

- continue until we find e_{2i+1} with $F \cup \{e_{2i+1}\} \in \mathcal{F}_1 \cap \mathcal{F}_2$



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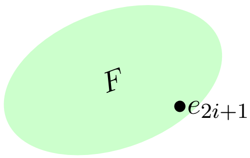

Intersection Algorithm: Idea

- *augmenting sequence/augmentation*: alternating insertion and deletion/complementary addition and subtraction
- sequences $x_0, y_1 ..., y_i, x_i$ with $F \cup \{x_0, ..., x_i\} \setminus \{y_1, ..., y_i\} \in \mathcal{F}_1 \cap \mathcal{F}_2$
- how to find?

Intersection Algorithm: Idea

- define auxiliary graph G_X with vertices E and find path between
  - $S_X = \{y.\ y \in E \setminus X \wedge X \cup \{y\} \in \mathcal{F}_1\}$
  - $T_X = \{y.\ y \in E \setminus X \wedge X \cup \{y\} \in \mathcal{F}_2\}$

  for $X \in \mathcal{F}_1 \cap \mathcal{F}_2$
- edges omitted
- involves various oracles
- shortest paths $x_0 y_1 x_1 \dots y_k x_k$ between S_X and T_X are augmenting paths, i.e. $X \setminus \{y_1, \dots, y_k\} \cup \{x_0, x_1, \dots, x_k\} \in \mathcal{F}_1 \cap \mathcal{F}_2$

Optimality Criterion

Theorem (Optimality Criterion by Korte and Vygen)

X is a set of maximum cardinality in $\mathcal{F}_1 \cap \mathcal{F}_2$ iff G_X does not contain a path from some $s \in S_X$ to some $t \in T_X$.

```
definition is-max X = (indep1 X  ∧  indep2 X  ∧
   (∄ Y. indep1 Y  ∧  indep2 Y  ∧  card Y > card X))

theorem maximum-characterisation:
  is-max X  ⟷
   ¬ (∃ p x y. x ∈ S  ∧  y ∈ T  ∧
     (vwalk-bet (A1  ∪  A2) x p y ∨ x = y))
```

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Algorithm 2: MaxMatroidIntersection(E, $\mathcal{F}_1$, $\mathcal{F}_2$)
[Lawler 1975, Korte and Vygen]

Initialise $X \leftarrow \emptyset$;
while $True$ **do**
  compute G_X*:* Initialise $S_X \leftarrow \emptyset$; $T_X \leftarrow \emptyset$; $A_{X,1} \leftarrow \emptyset$; $A_{X,2} \leftarrow \emptyset$;
  for $y \in E \setminus X$ **do**
    if $X \cup \{y\} \in \mathcal{F}_1$ **then** $S_X \leftarrow S_X \cup \{y\}$;
    else for $x \in X$ **do** [**if** $X \setminus \{x\} \cup \{y\} \in \mathcal{F}_1$ **then** $A_{X,1} \leftarrow A_{X,1} \cup \{(x, y)\}$;]
    if $X \cup \{y\} \in \mathcal{F}_2$ **then** $T_X \leftarrow T_X \cup \{y\}$;
    else for $x \in X$ **do** [**if** $X \setminus \{x\} \cup \{y\} \in \mathcal{F}_2$ **then** $A_{X,2} \leftarrow A_{X,2} \cup \{(y, x)\}$;]
  if $\exists$ *path leading from* S_X *to* T_X *via the edges in* $A_{X,1} \cup A_{X,2}$ **then**
    find a shortest path $P = x_0 y_1 x_1 \ldots y_s x_s$ leading from S_X to T_X;
    augment along P: $X \leftarrow X \cup \{x_0, \ldots, x_s\} \setminus \{y_1, \ldots, y_s\}$;
  else return X as maximum cardinality set in $\mathcal{F}_1 \cap \mathcal{F}_2$;

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- greedoids formalised for the first time

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- algorithmic characterisations of matroids and greedoids

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  - maximum flow: maximum flow iff $\nexists$ augmenting path (part of Maxflow-Mincut Theorem)
  - minimum cost flow: minimum costs iff $\nexists$ augmenting cycle
  - matching: maximum matching iff $\nexists$ augmenting path (Berge's Lemma)

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THANK YOU!

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