6.036/6.862: Introduction to Machine Learning

Lecture: starts Tuesdays 9:35am (Boston time zone)

Course website: introml.odl.mit.edu

Who's talking? Prof. Tamara Broderick

Questions? discourse.odl.mit.edu ("Lecture 3" category)

Materials: Will all be available at course website

Last Time(s)

I. Linear classifiers
II. Perceptron algorithm
III. Linear separability
IV. Perceptron theorem

Today's Plan

I. A more-complete ML analysis
II. Choosing good features
III. Evaluation

Recall

Recall

- Linear classifier h

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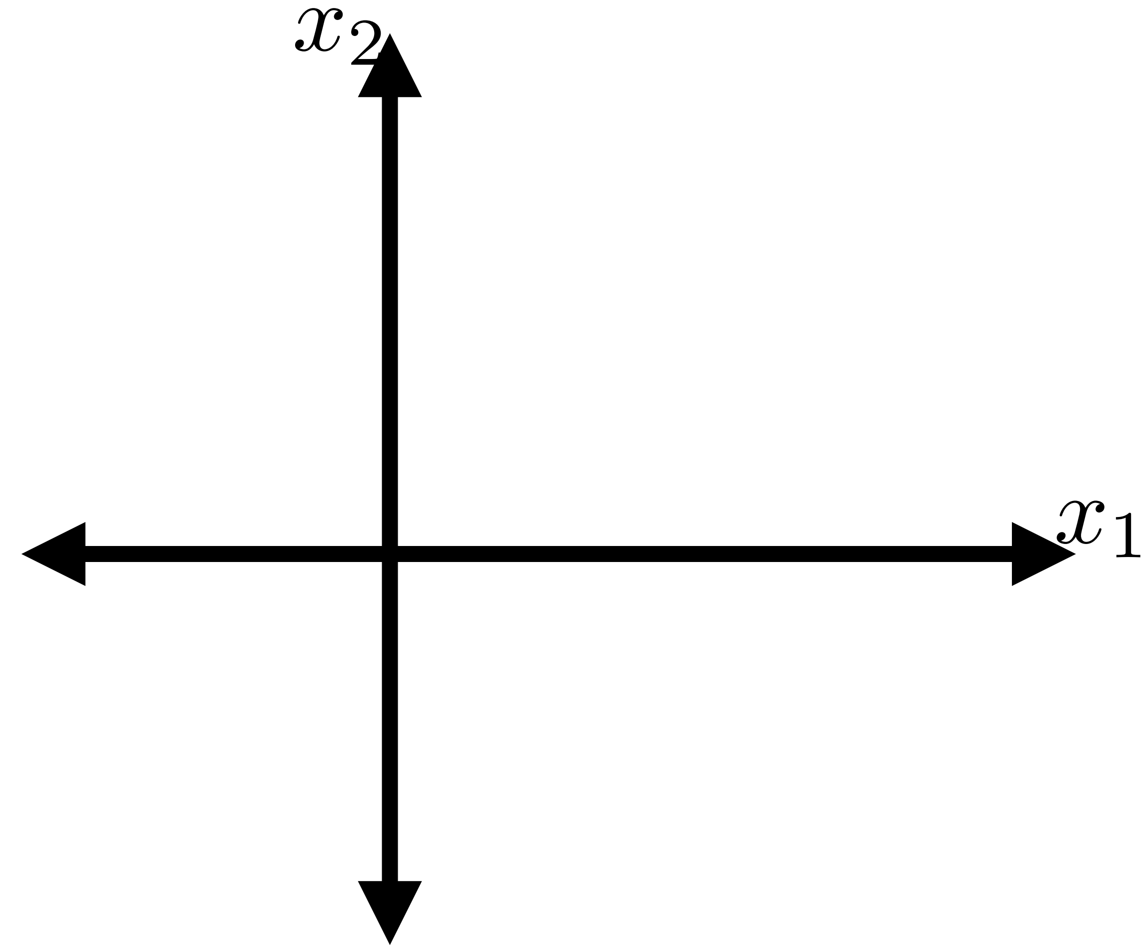

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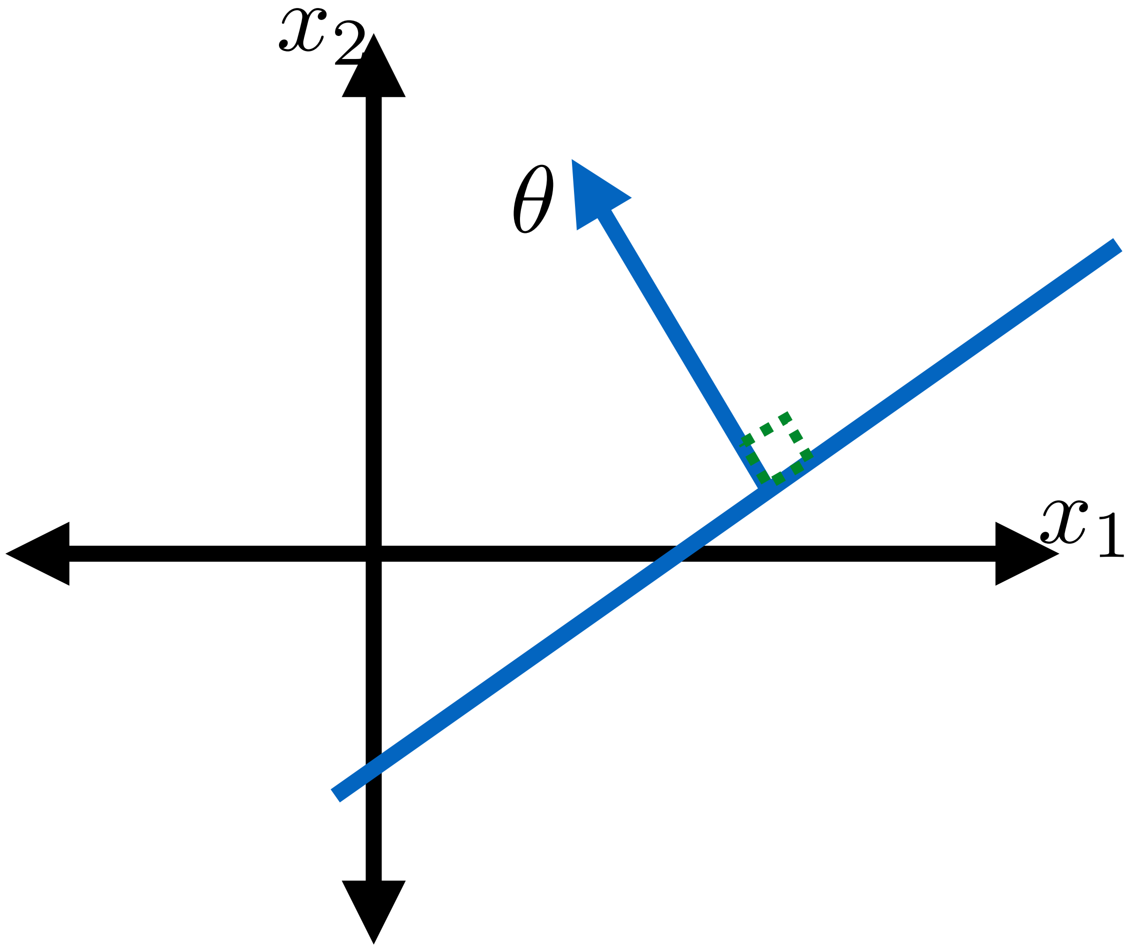

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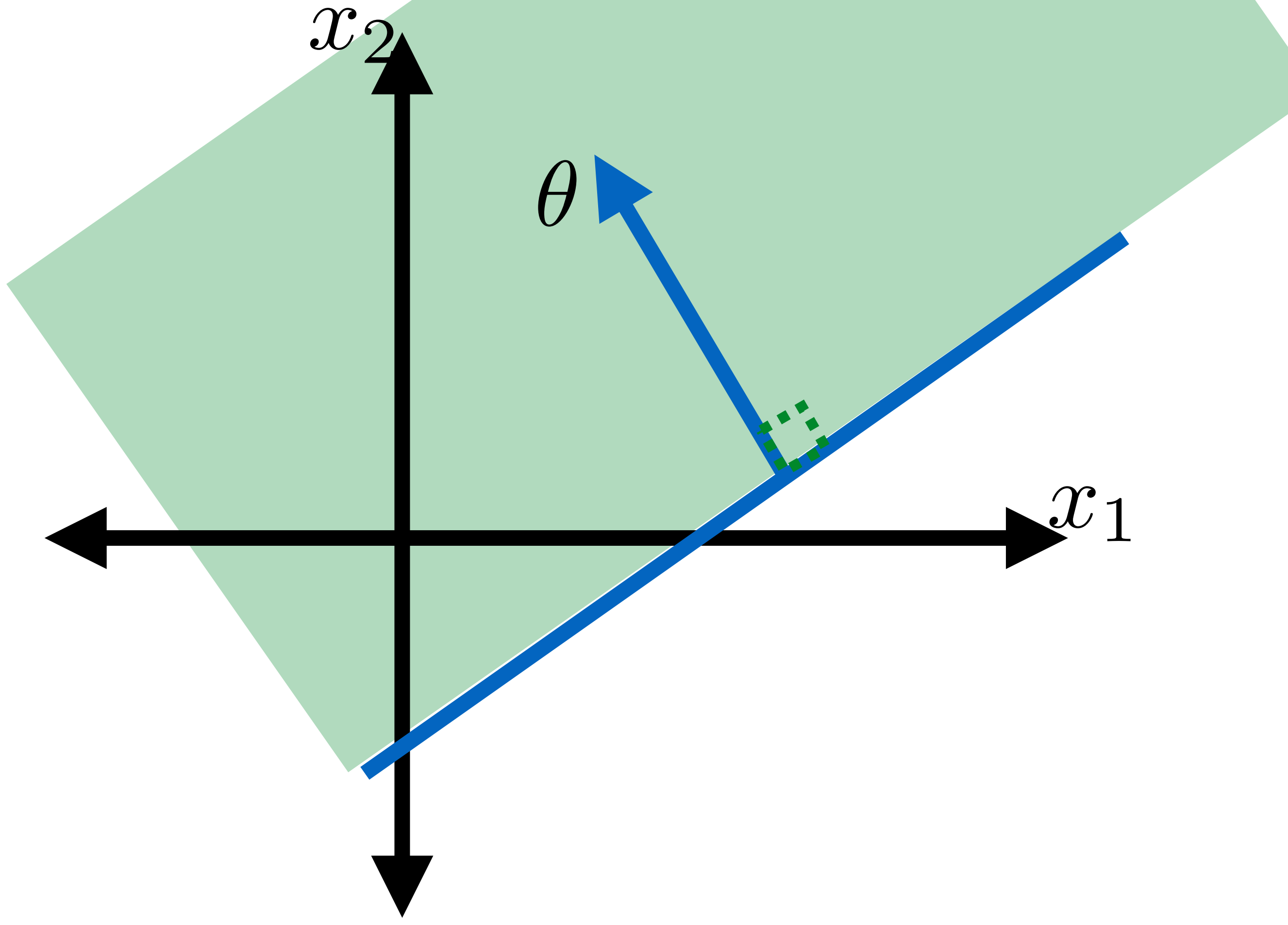

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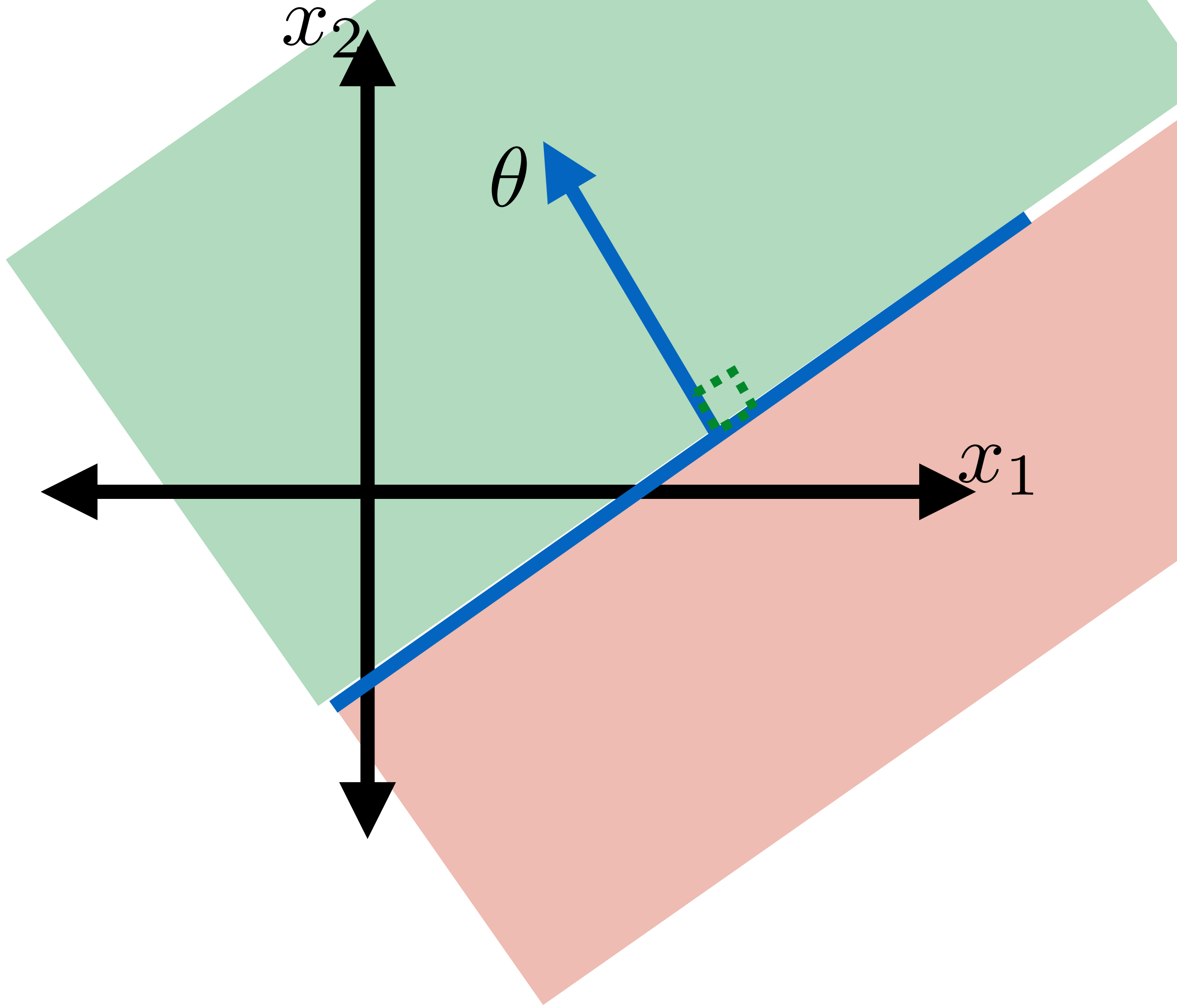

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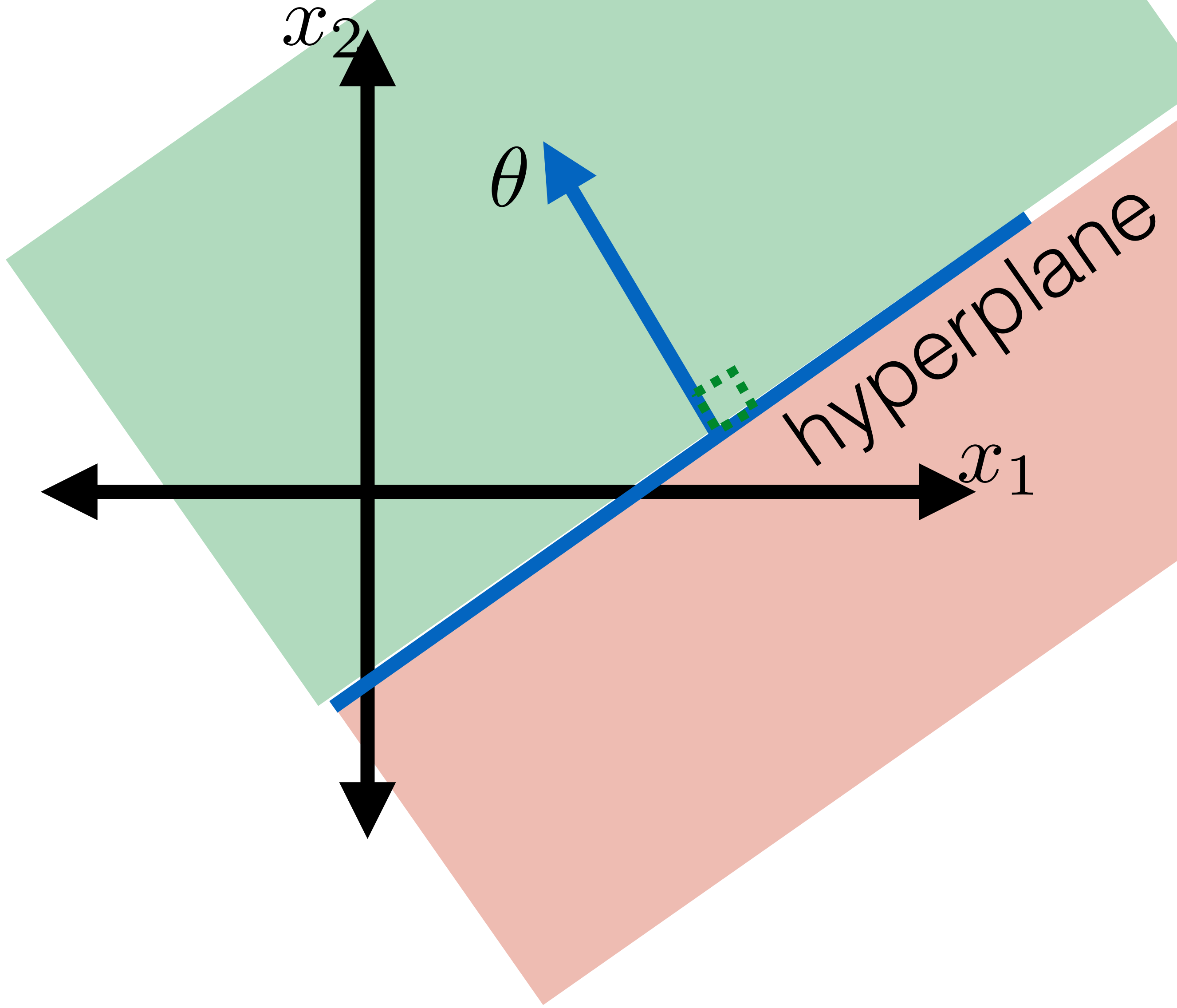

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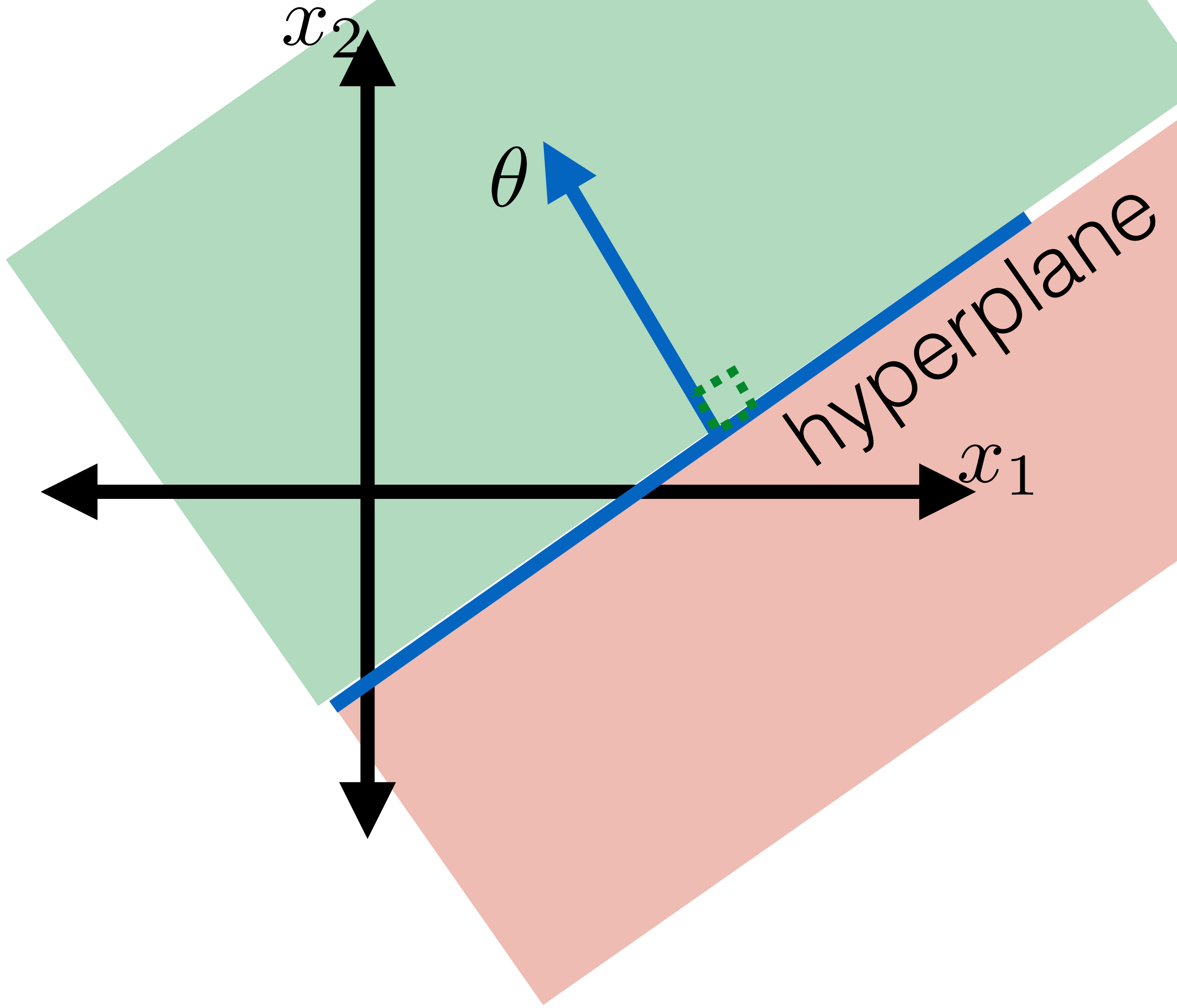

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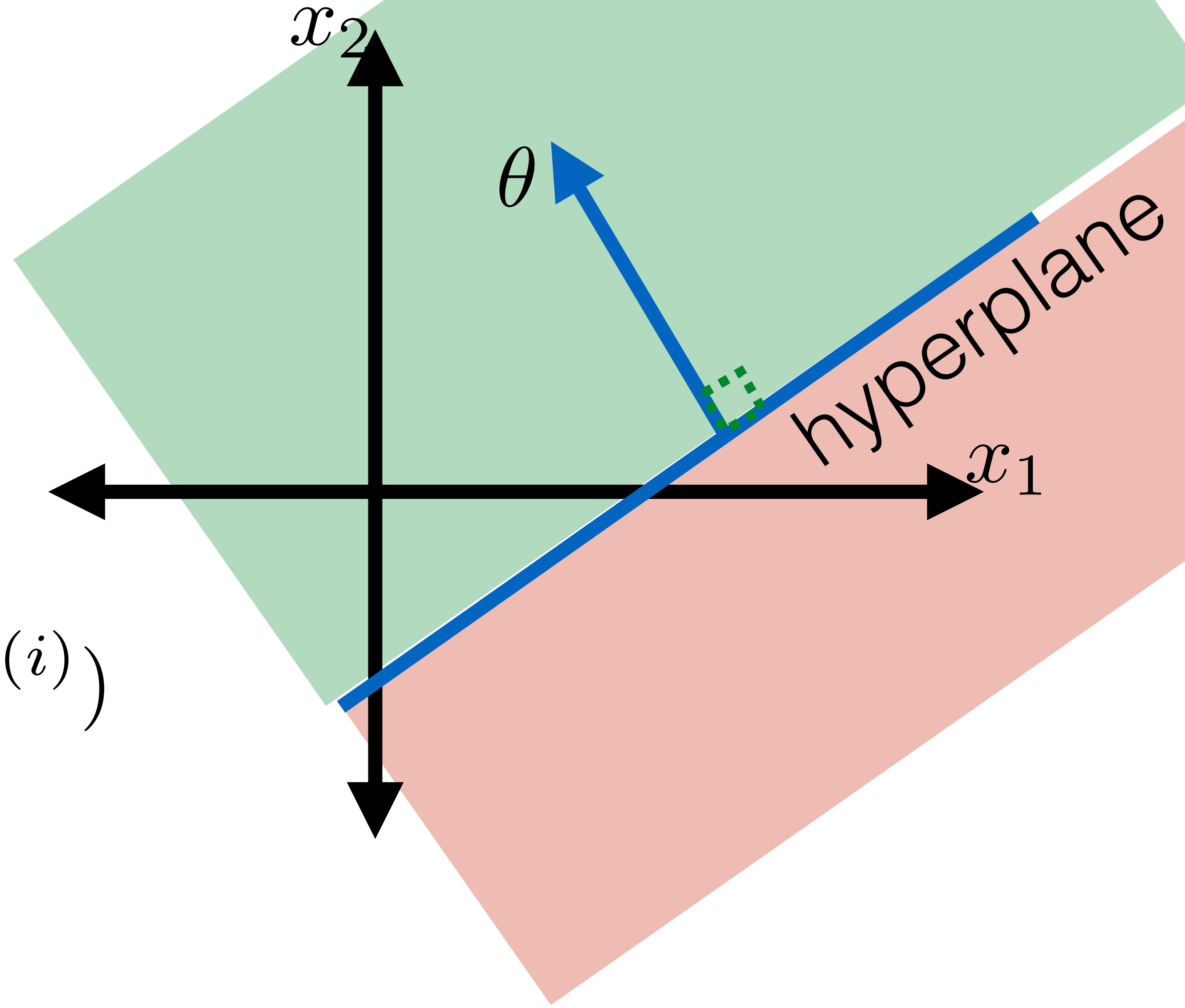

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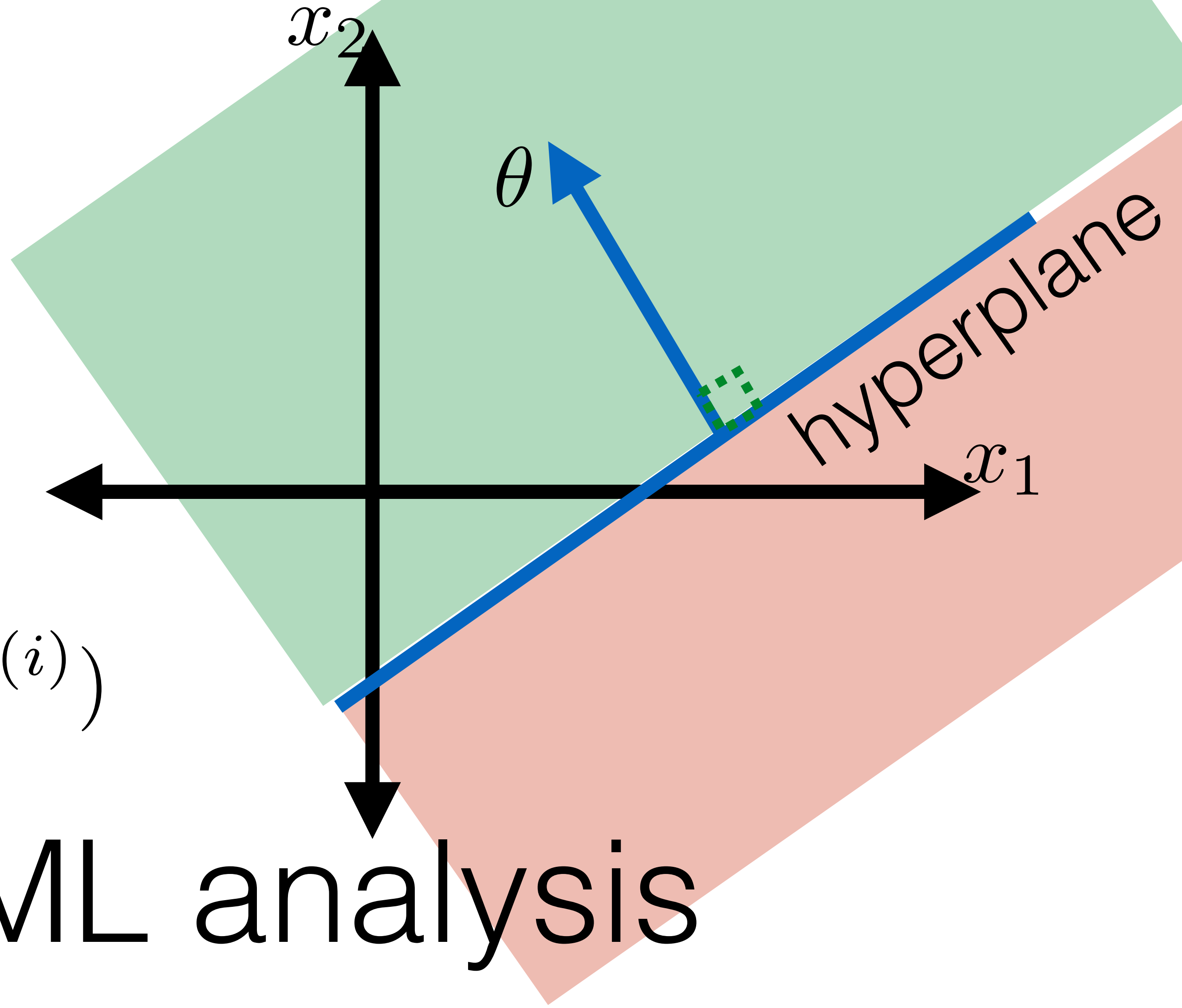

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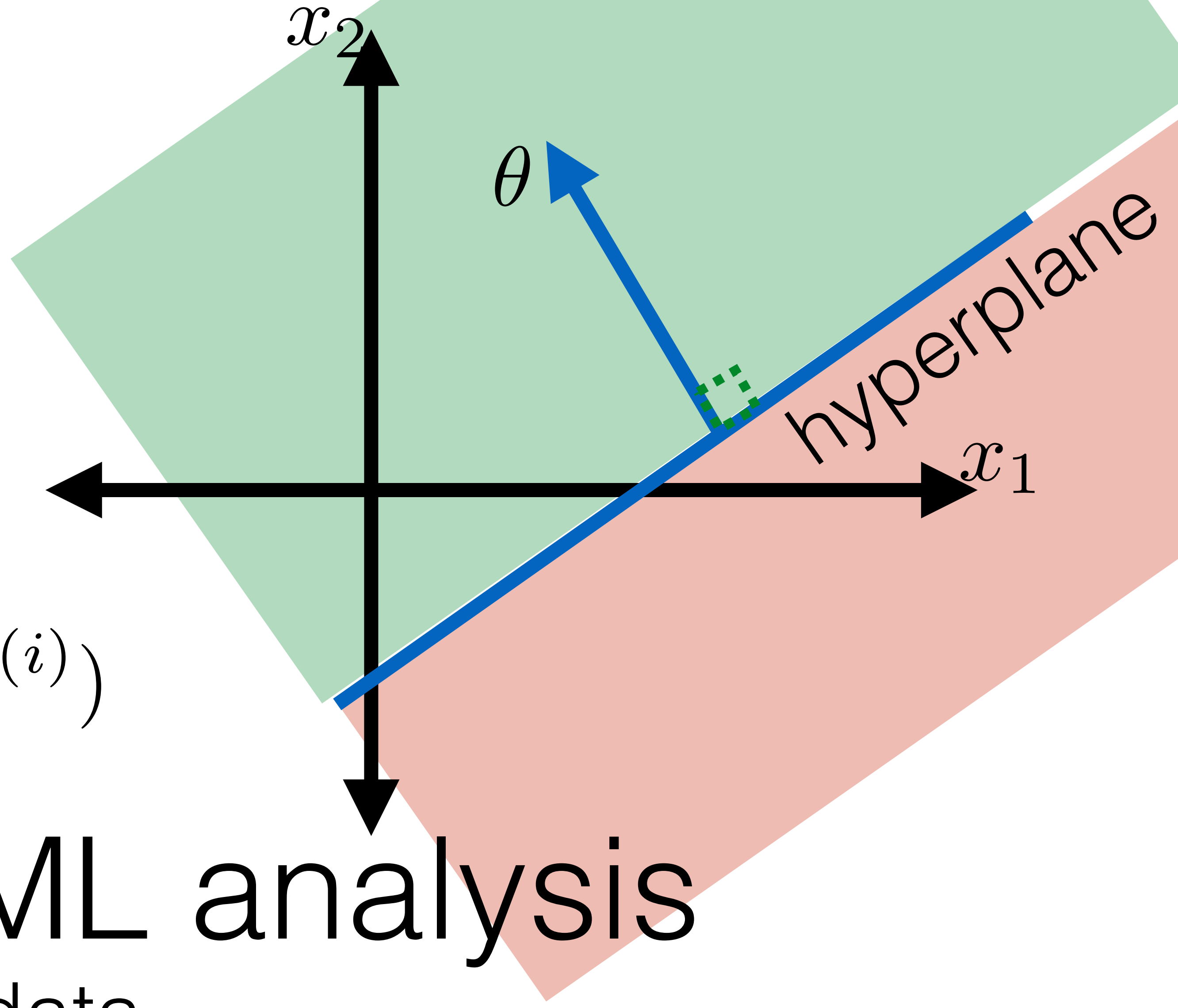

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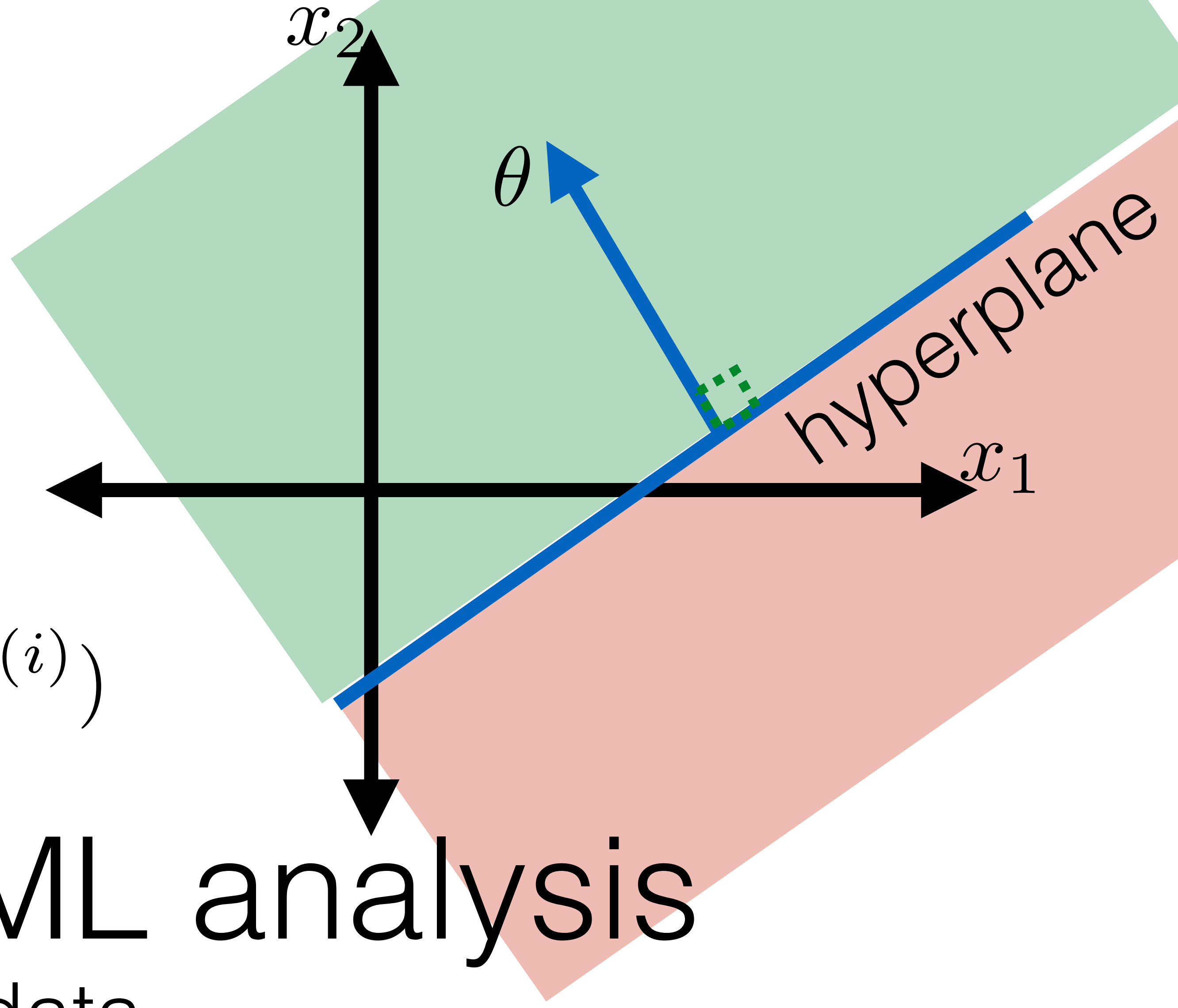

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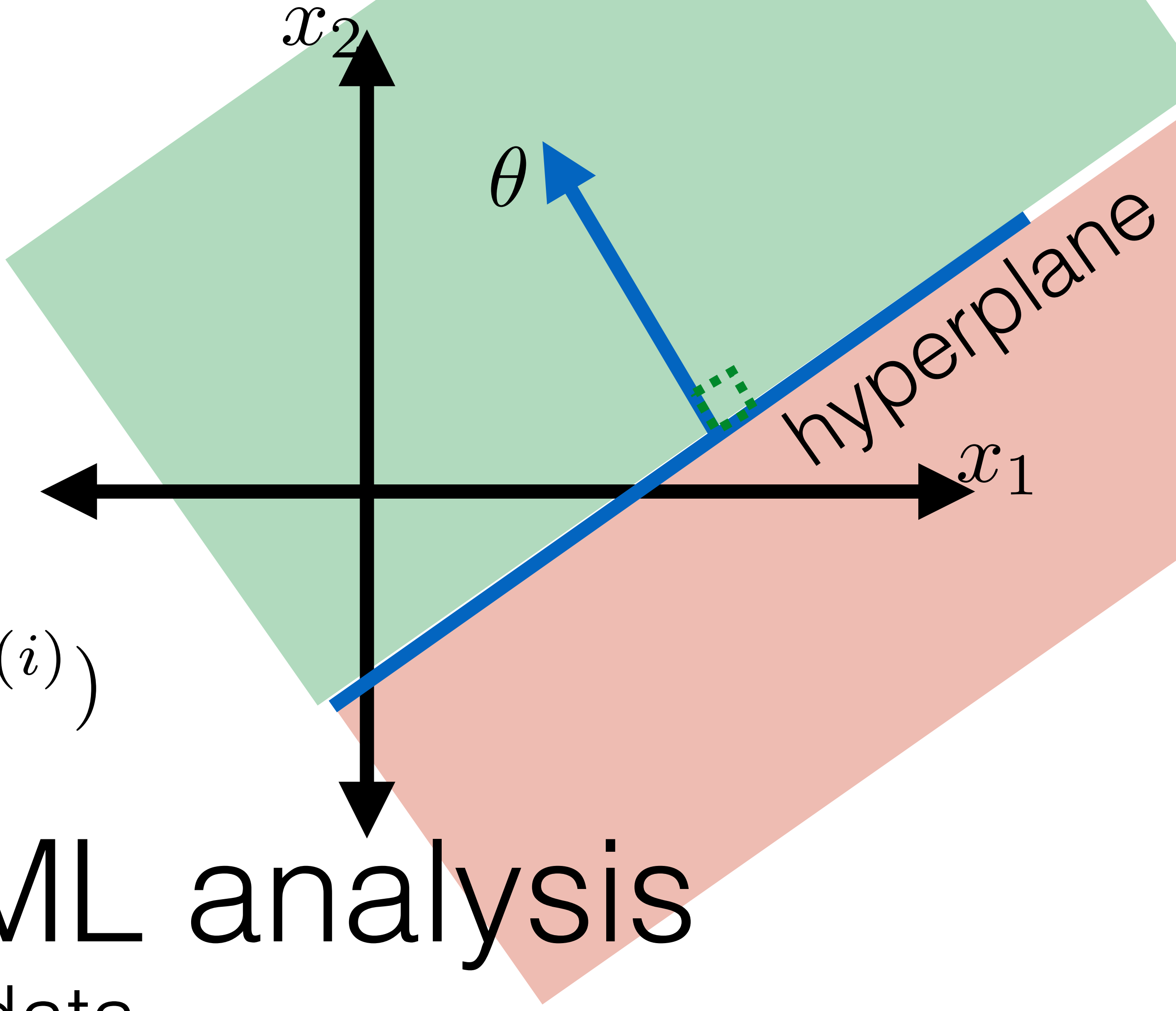

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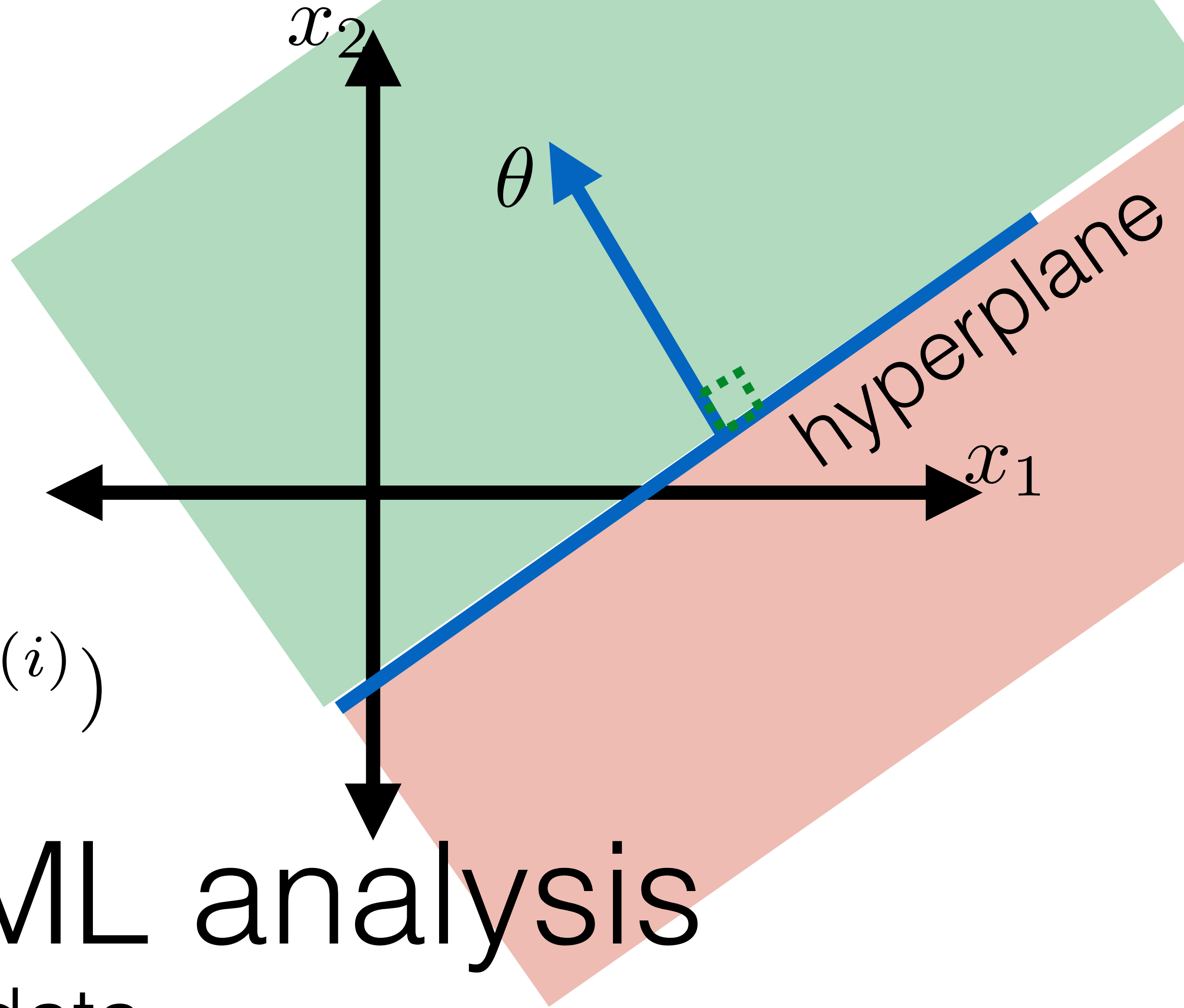

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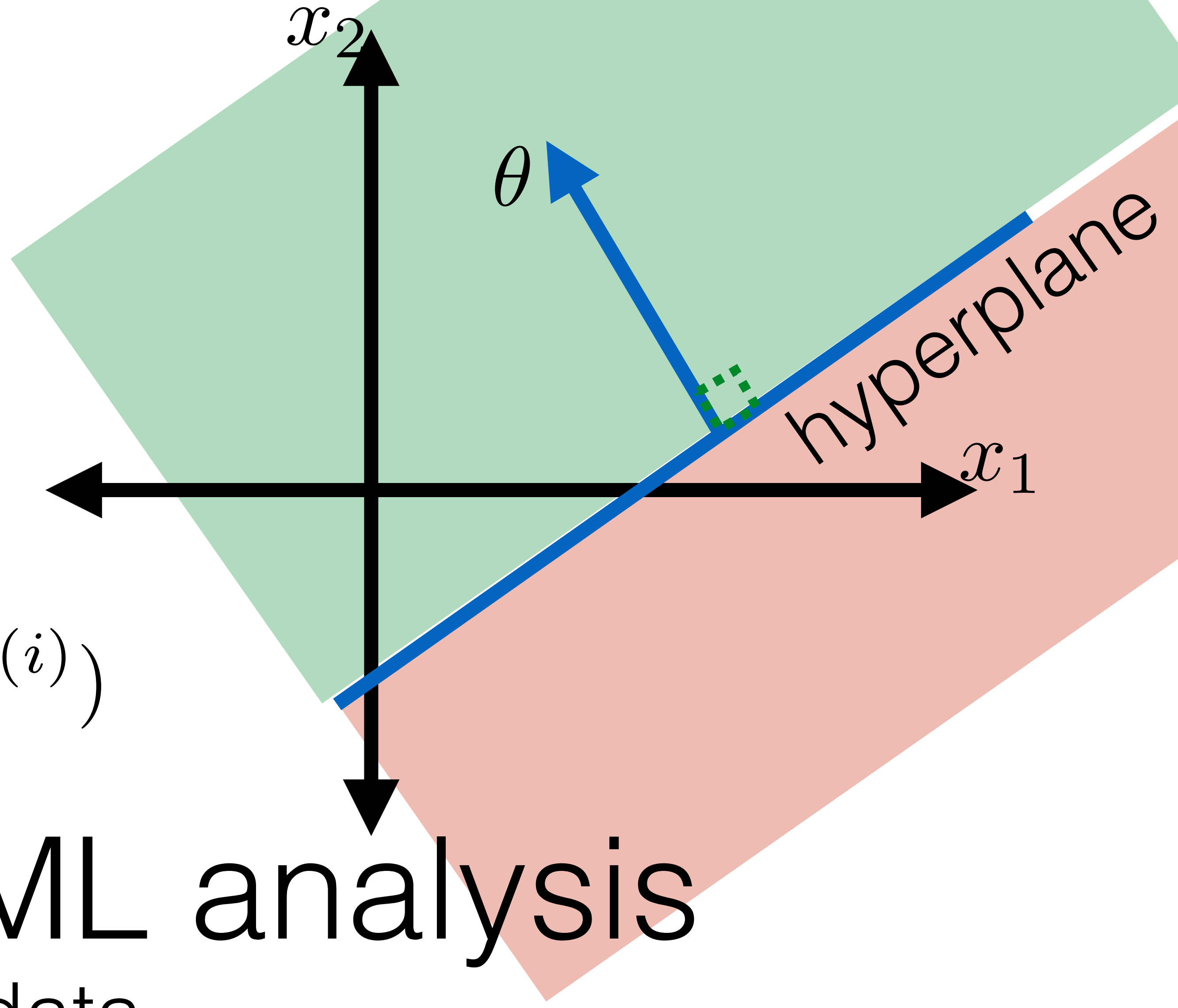

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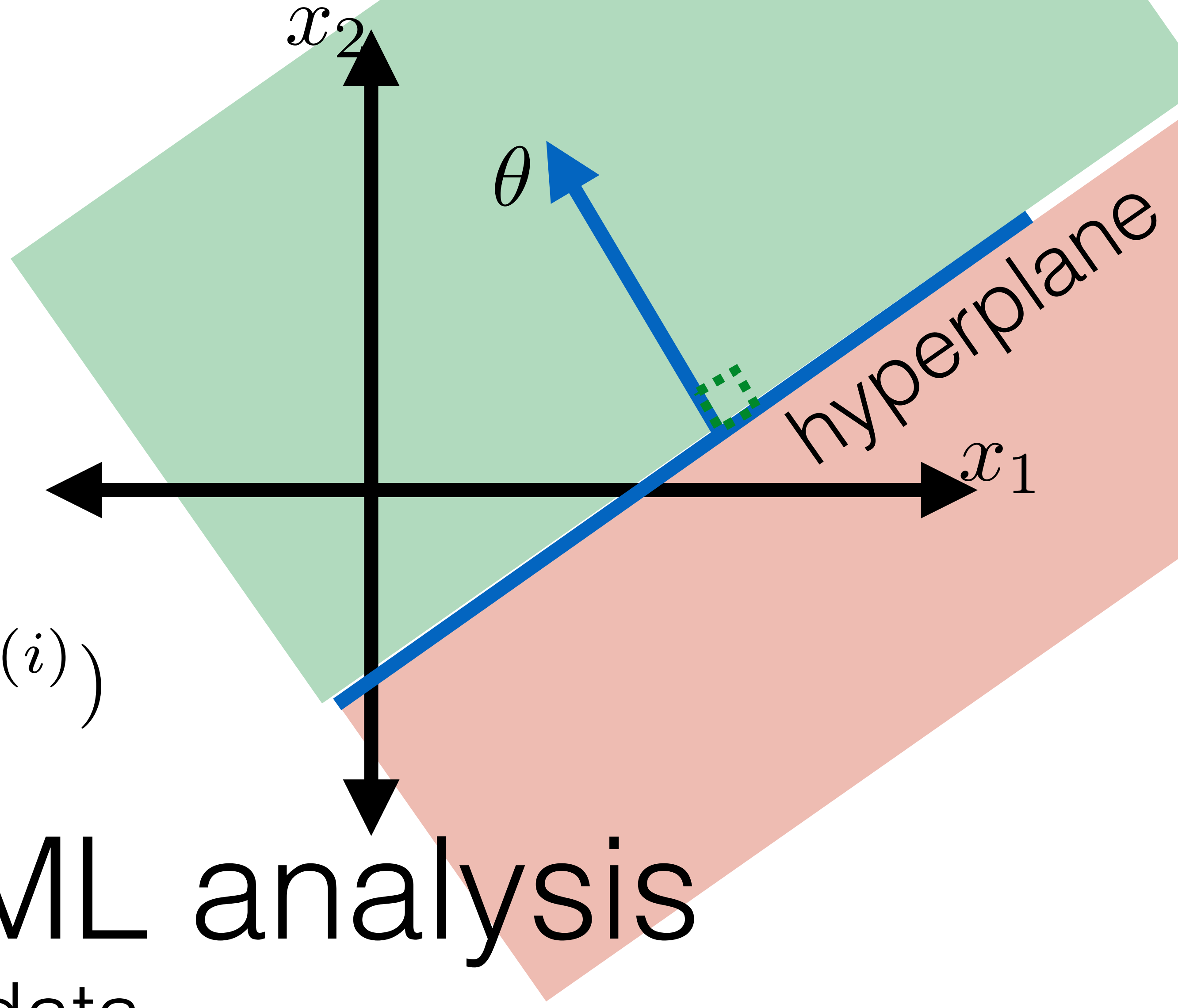

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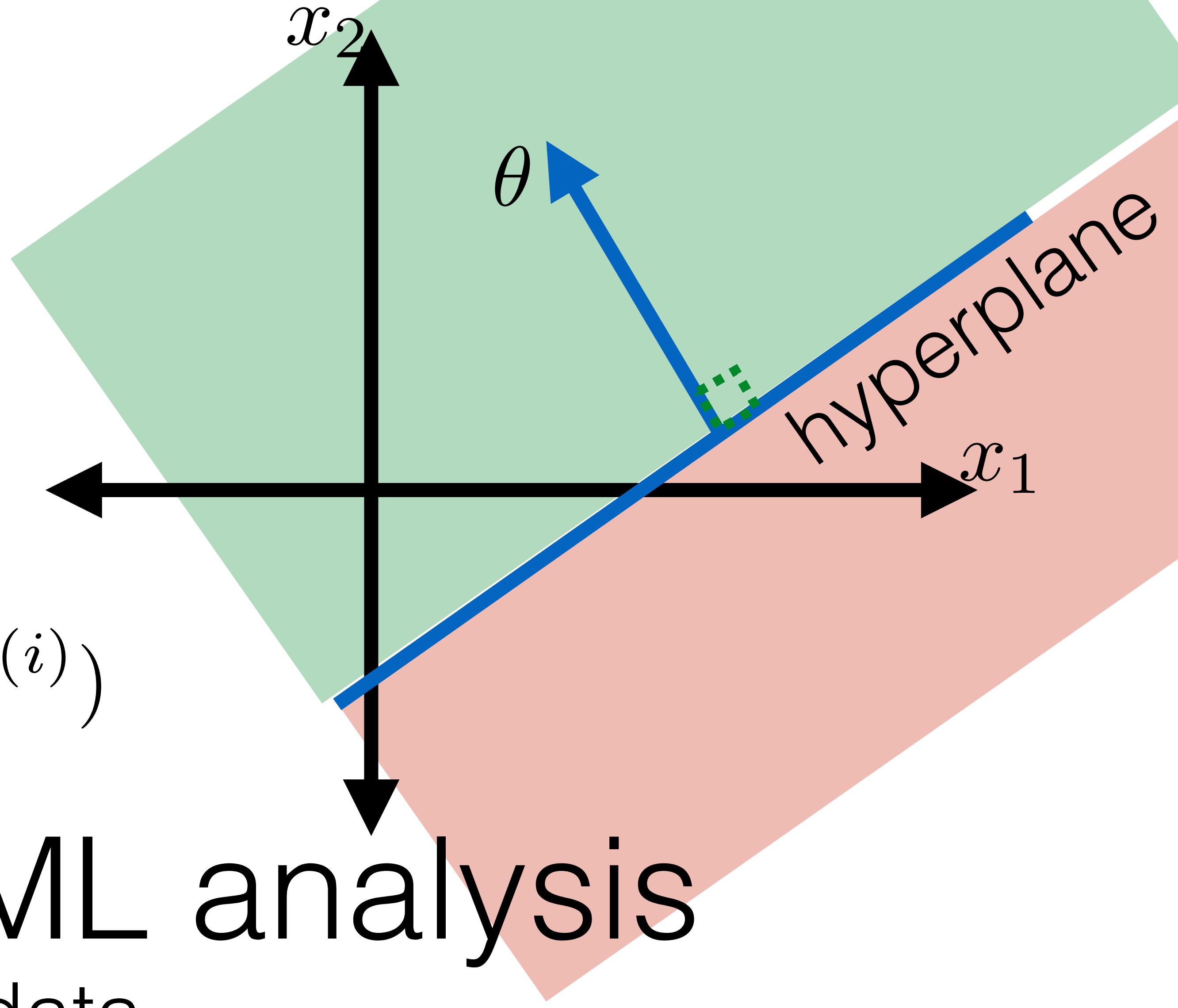

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4. Interpretation & evaluation

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2	no	71	no	admin	beta blockers, pain	20s	34000
3	yes	89	yes	nurse	beta blockers	50s	40000
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- Save mapping to recover predictions of new points

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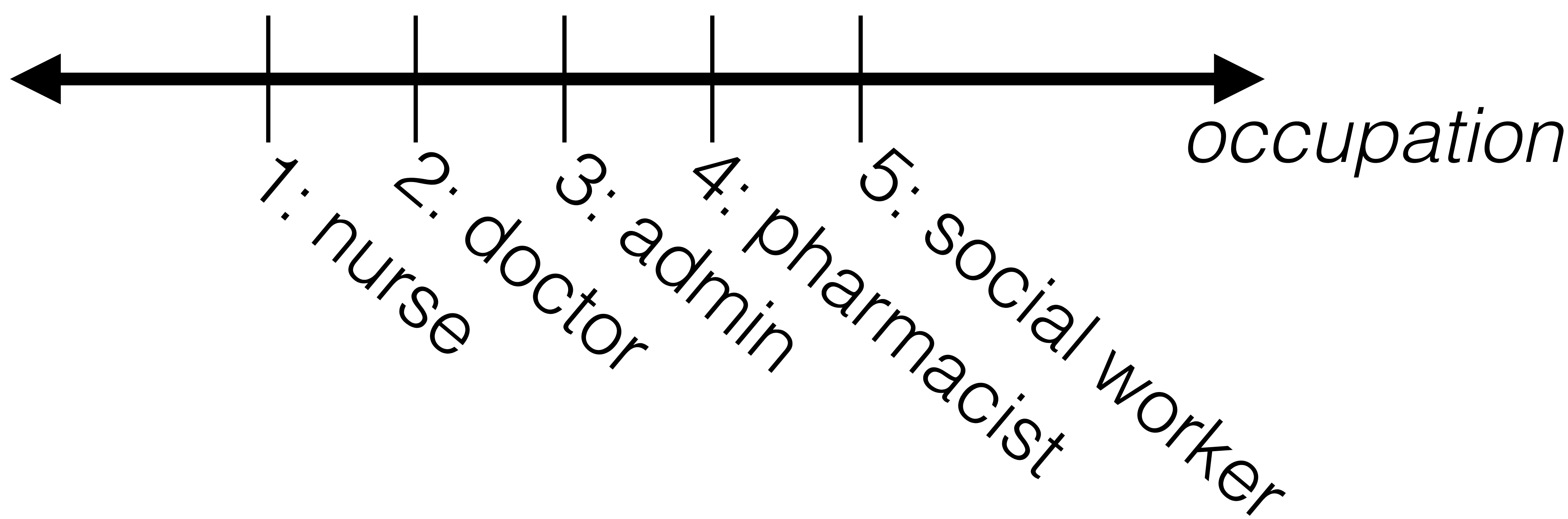

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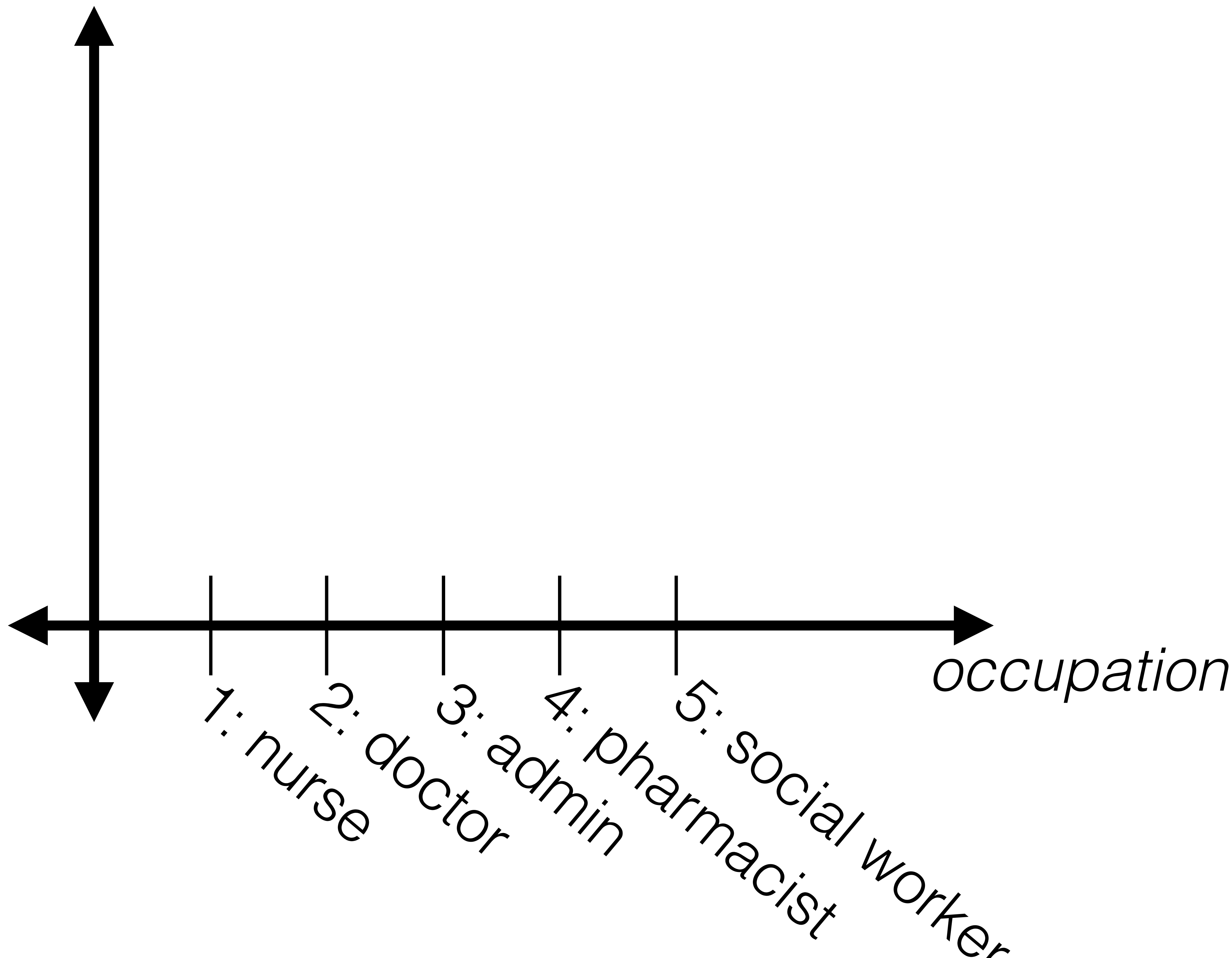

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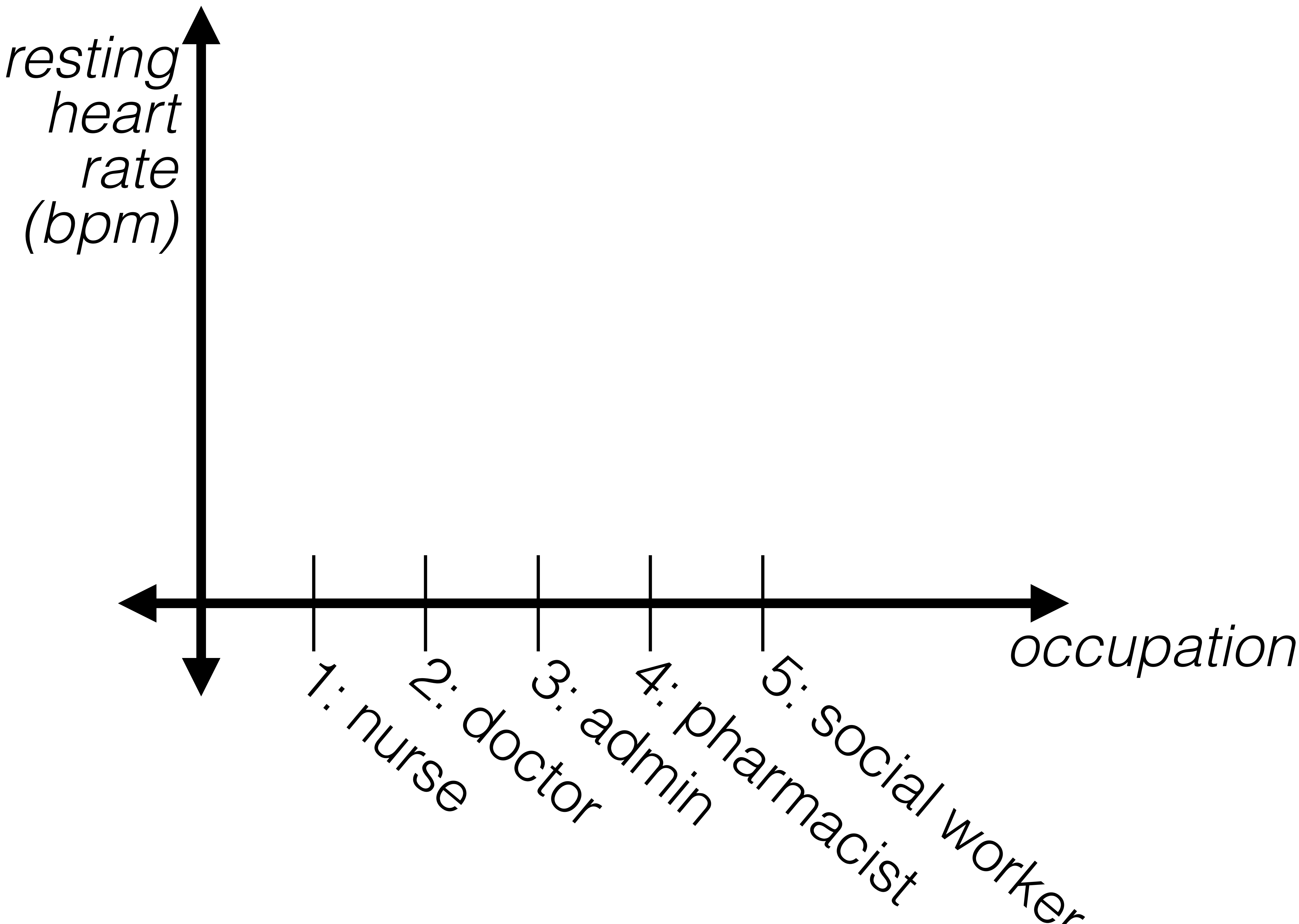

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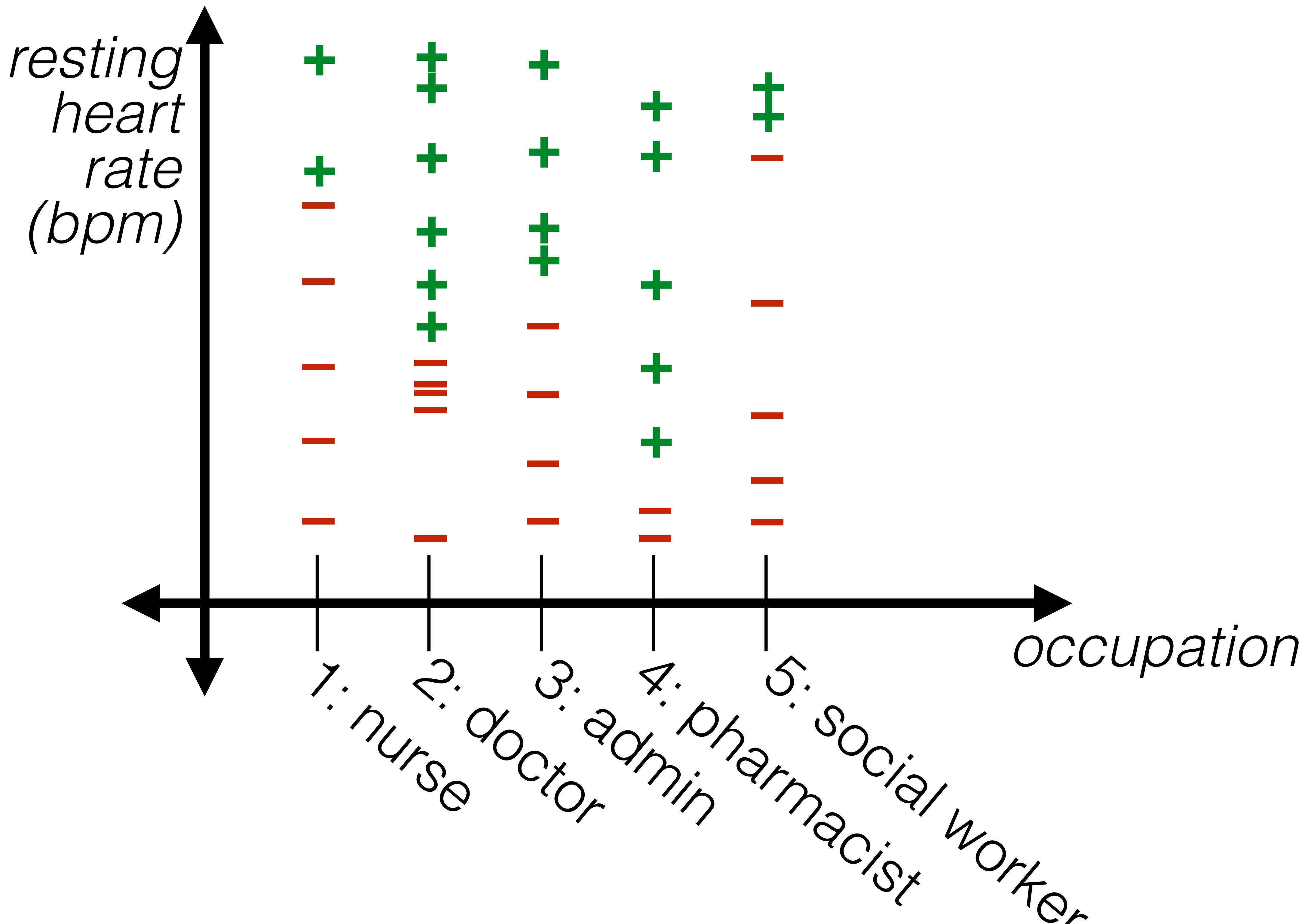

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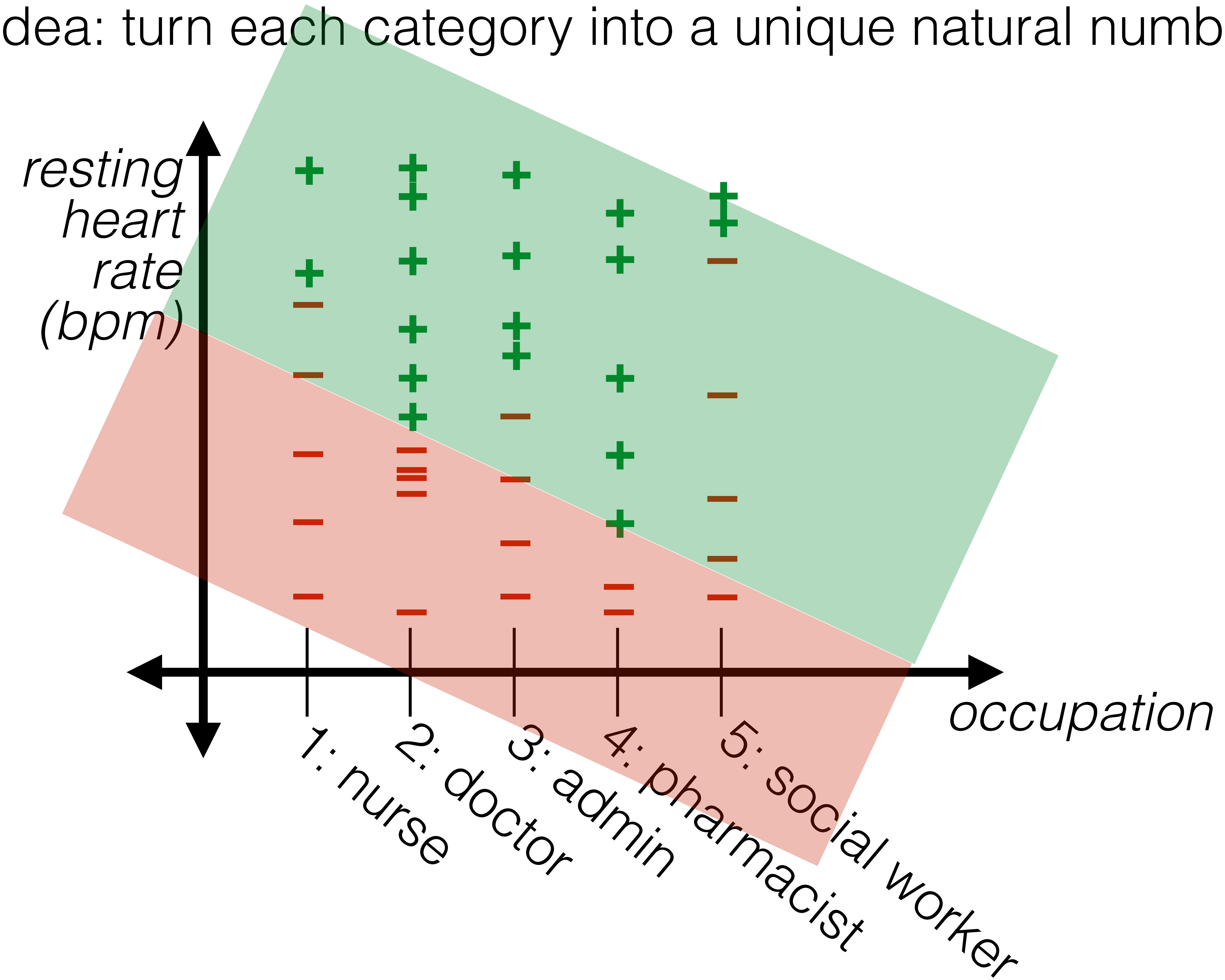

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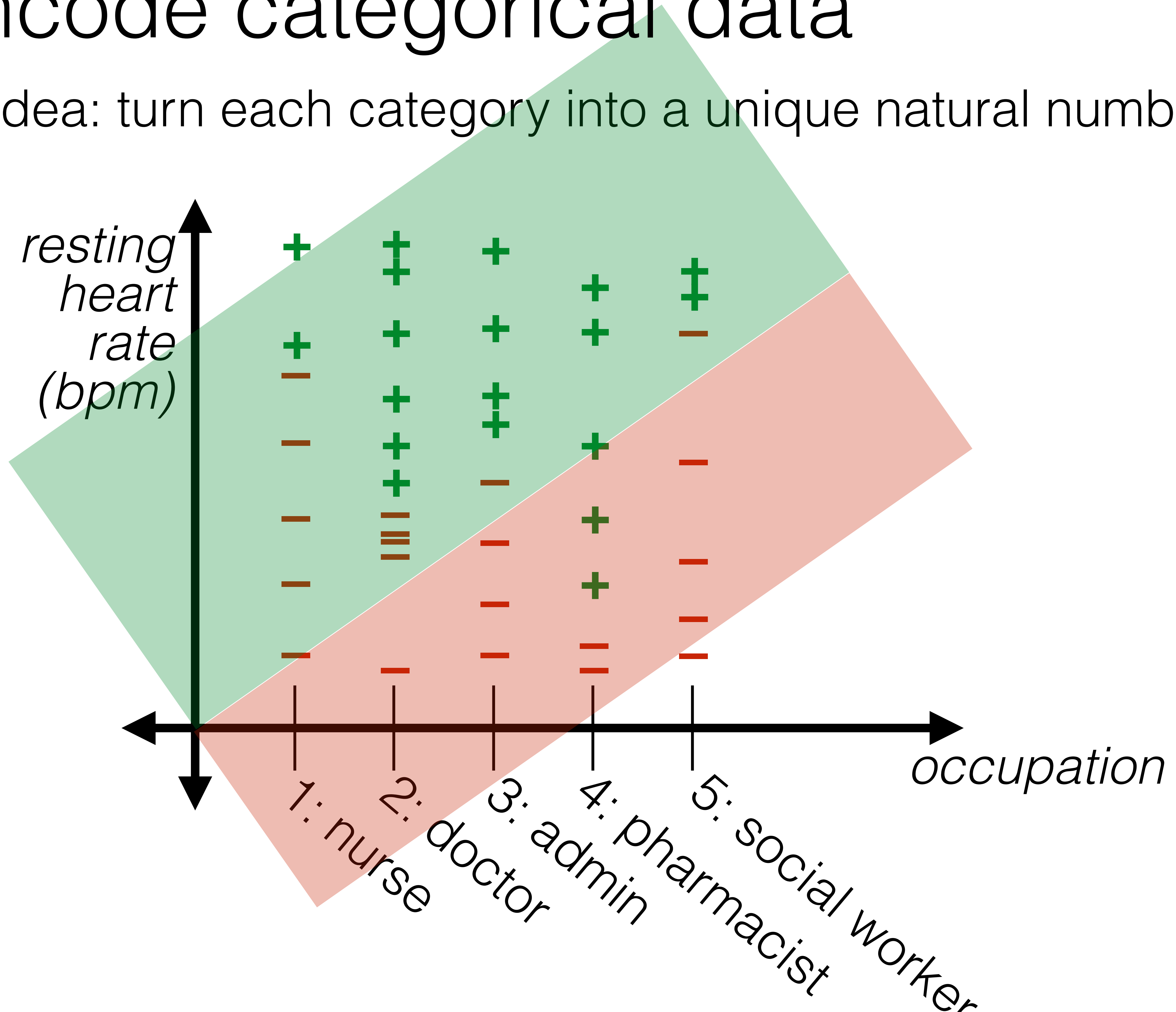

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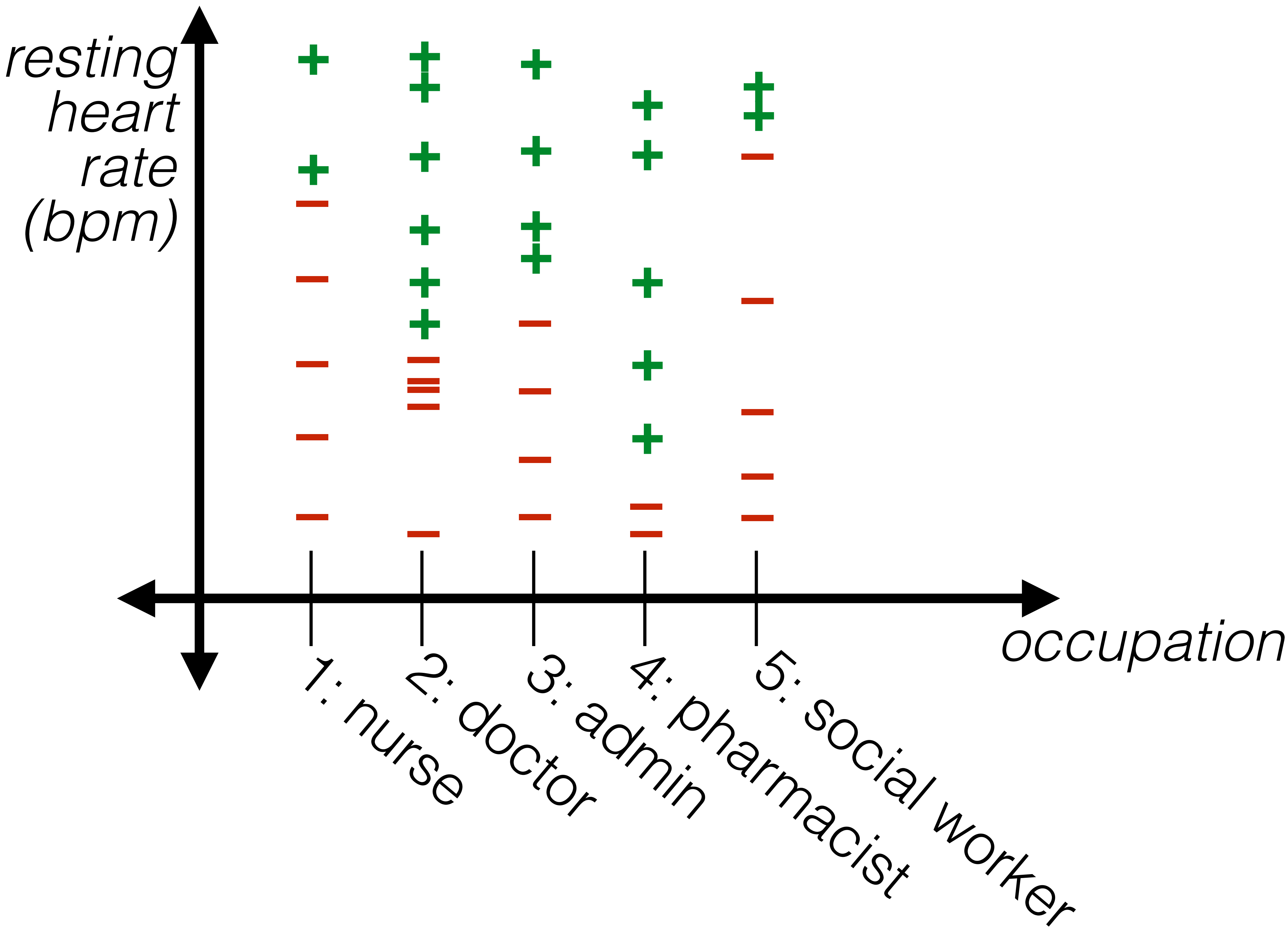

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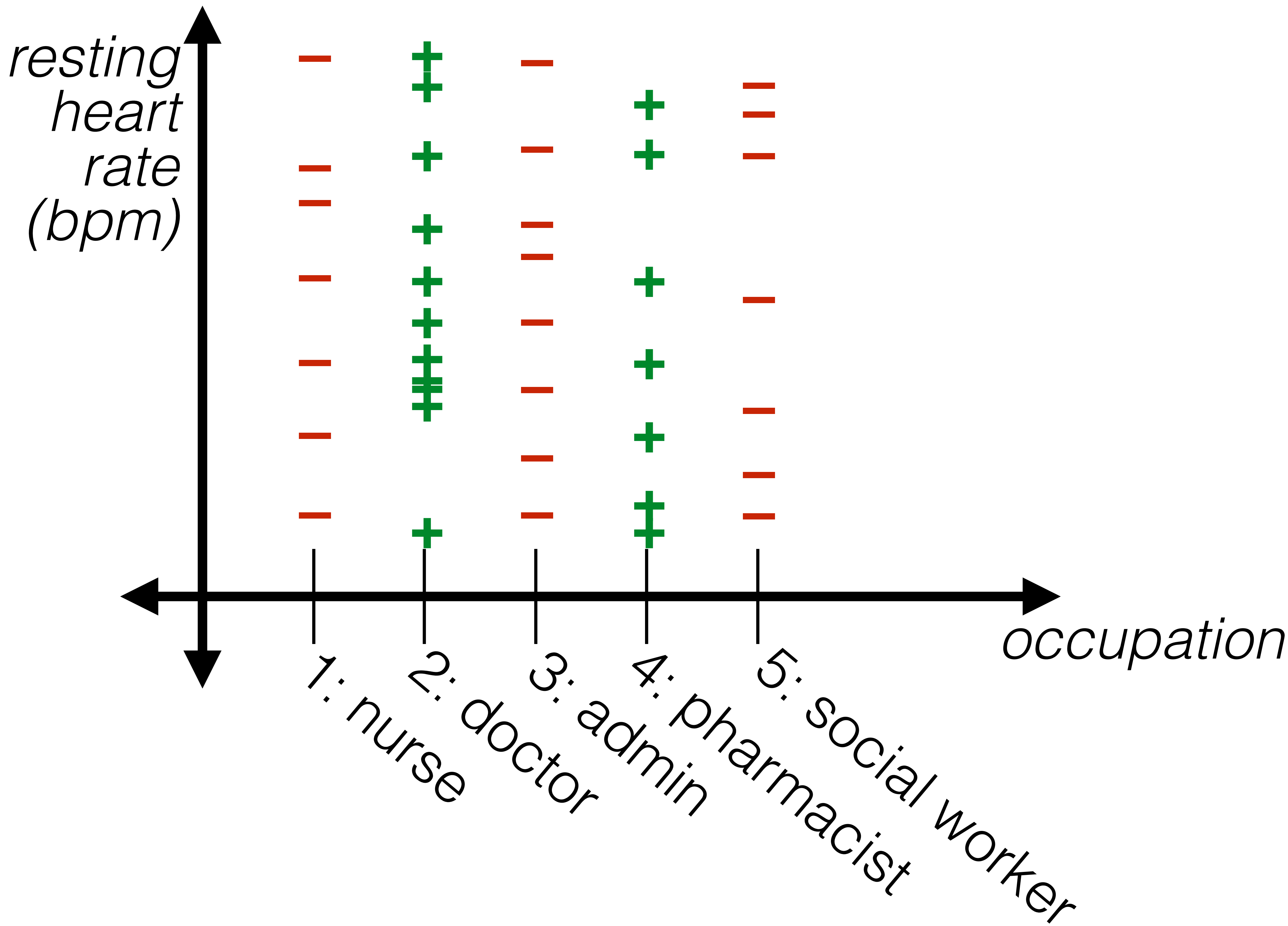

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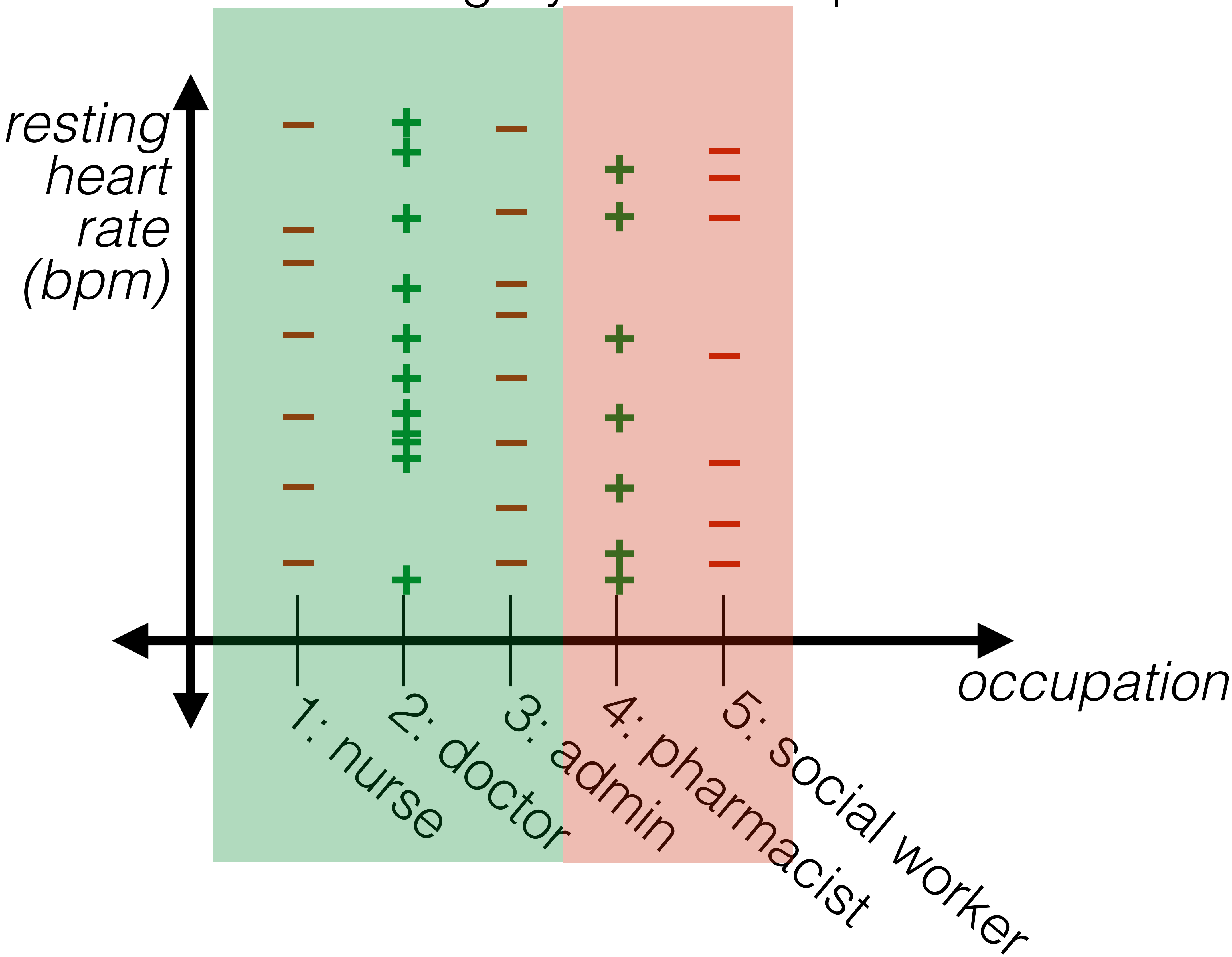

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pharmacist	0	1	0
doctor	0	1	1
social worker	1	0	0

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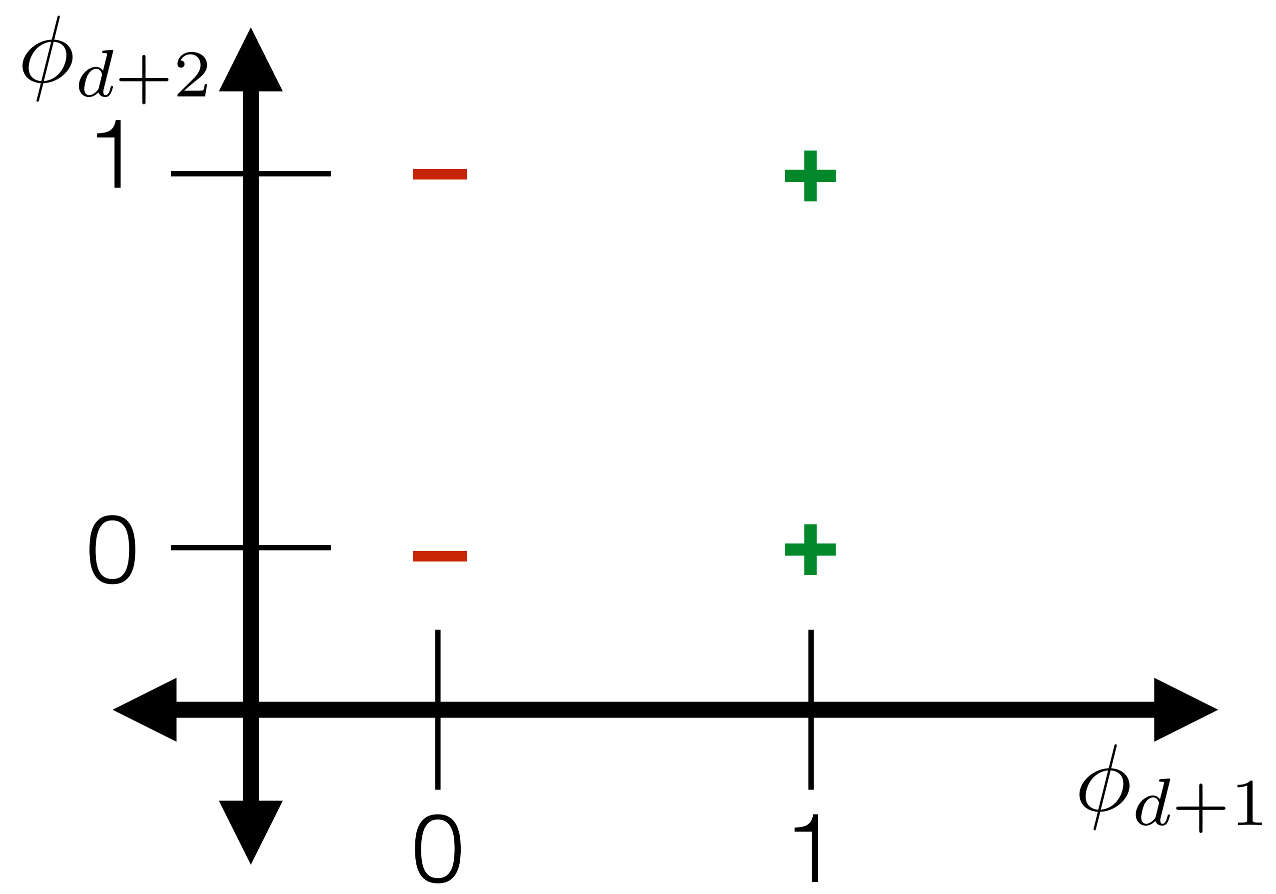

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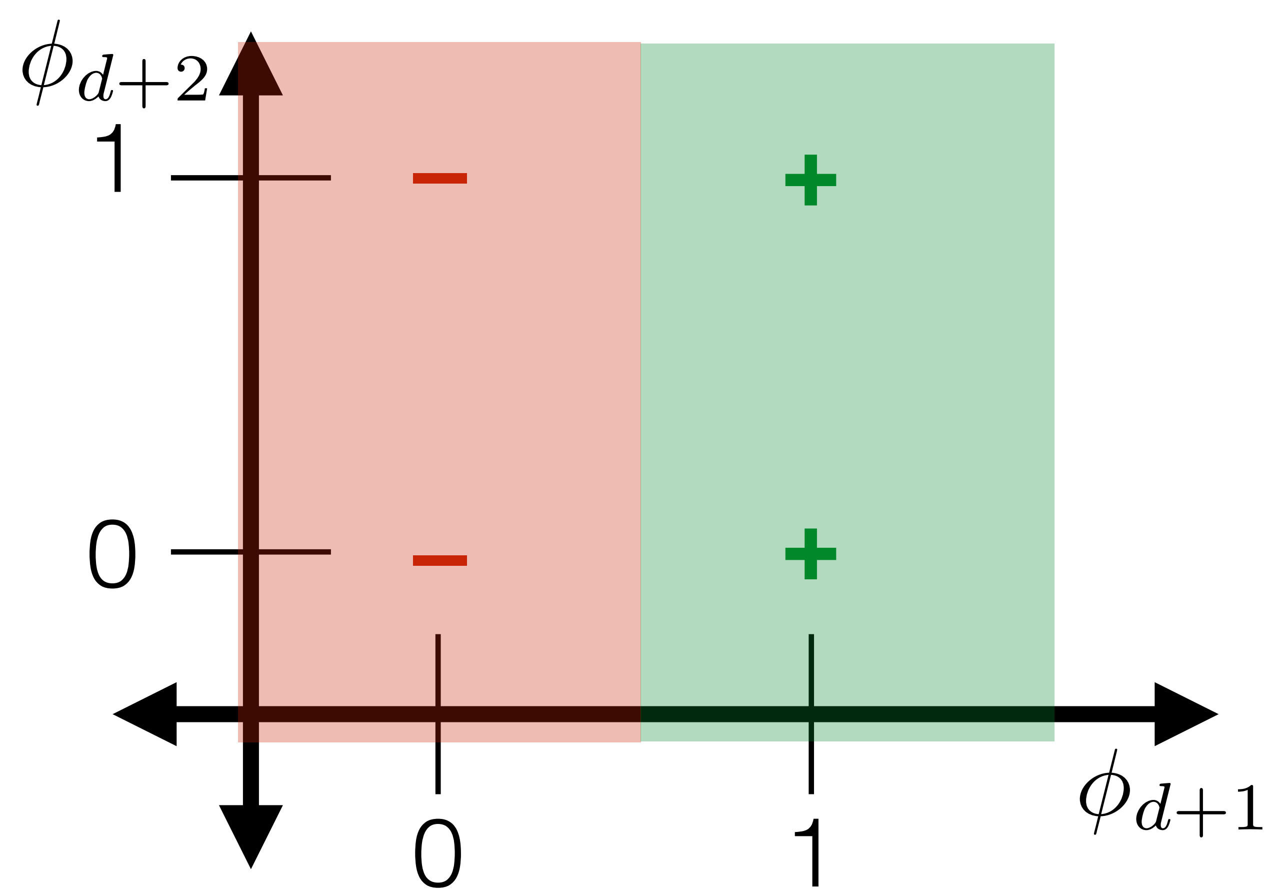

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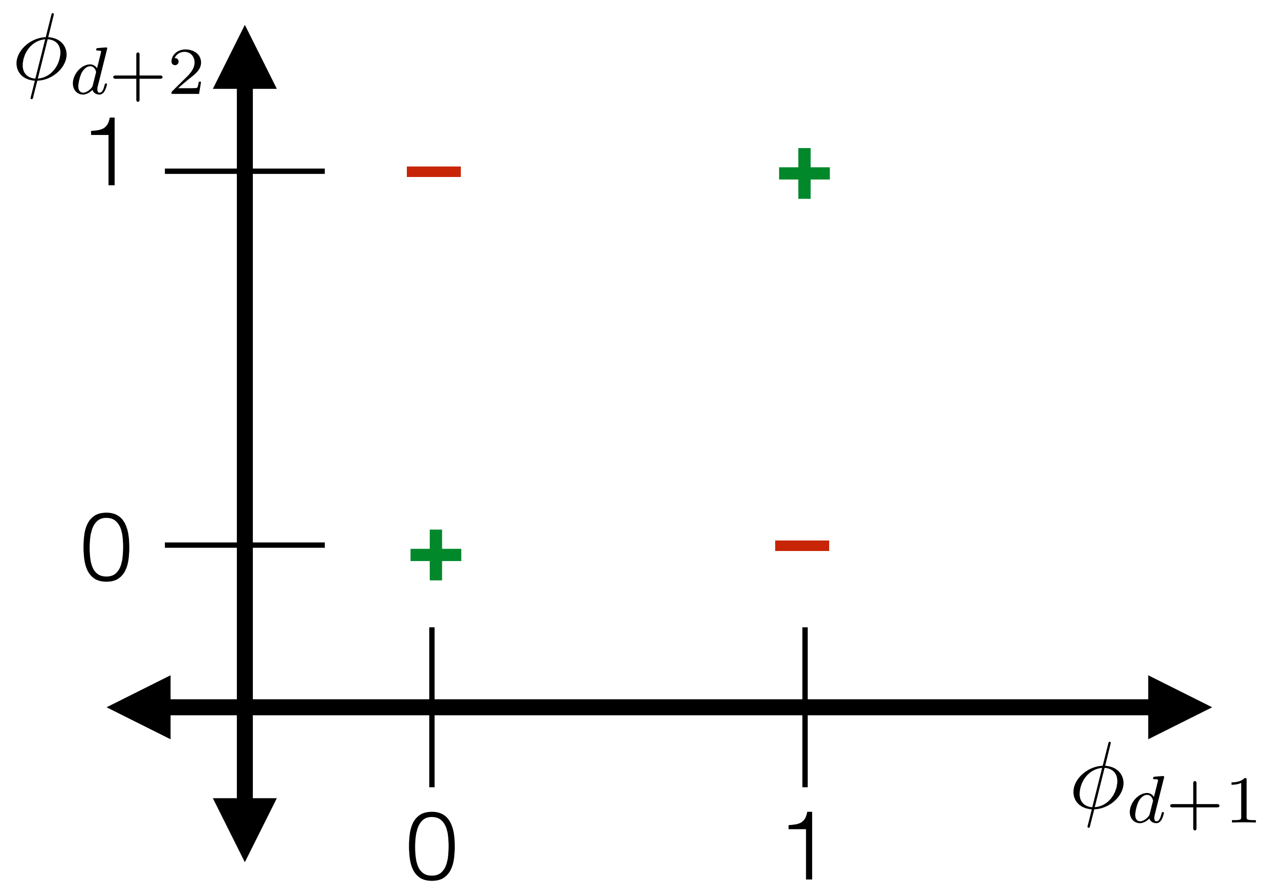

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doctor	0	0	0	1	0
social worker	0	0	0	0	1

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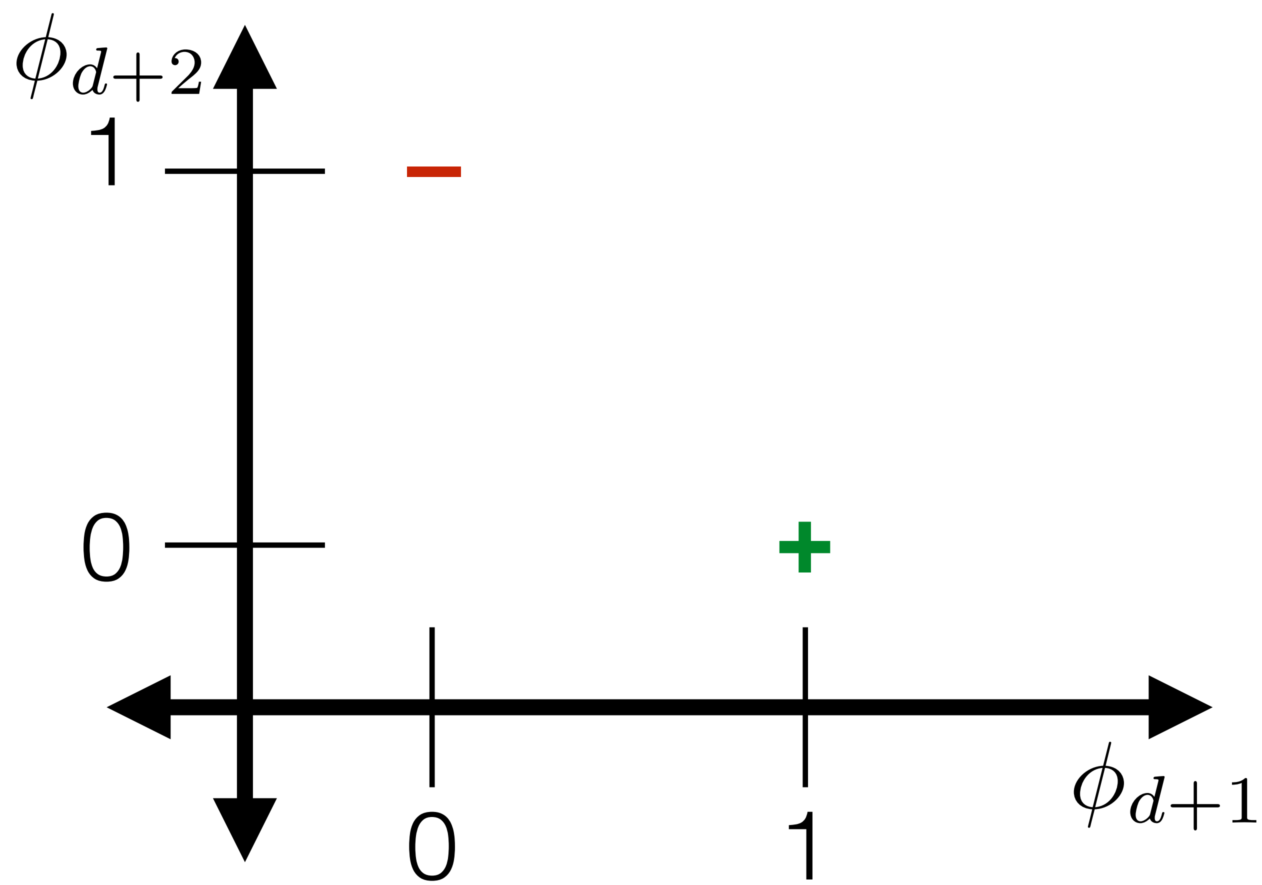
doctor	0	0	0	1	0
social worker	0	0	0	0	1

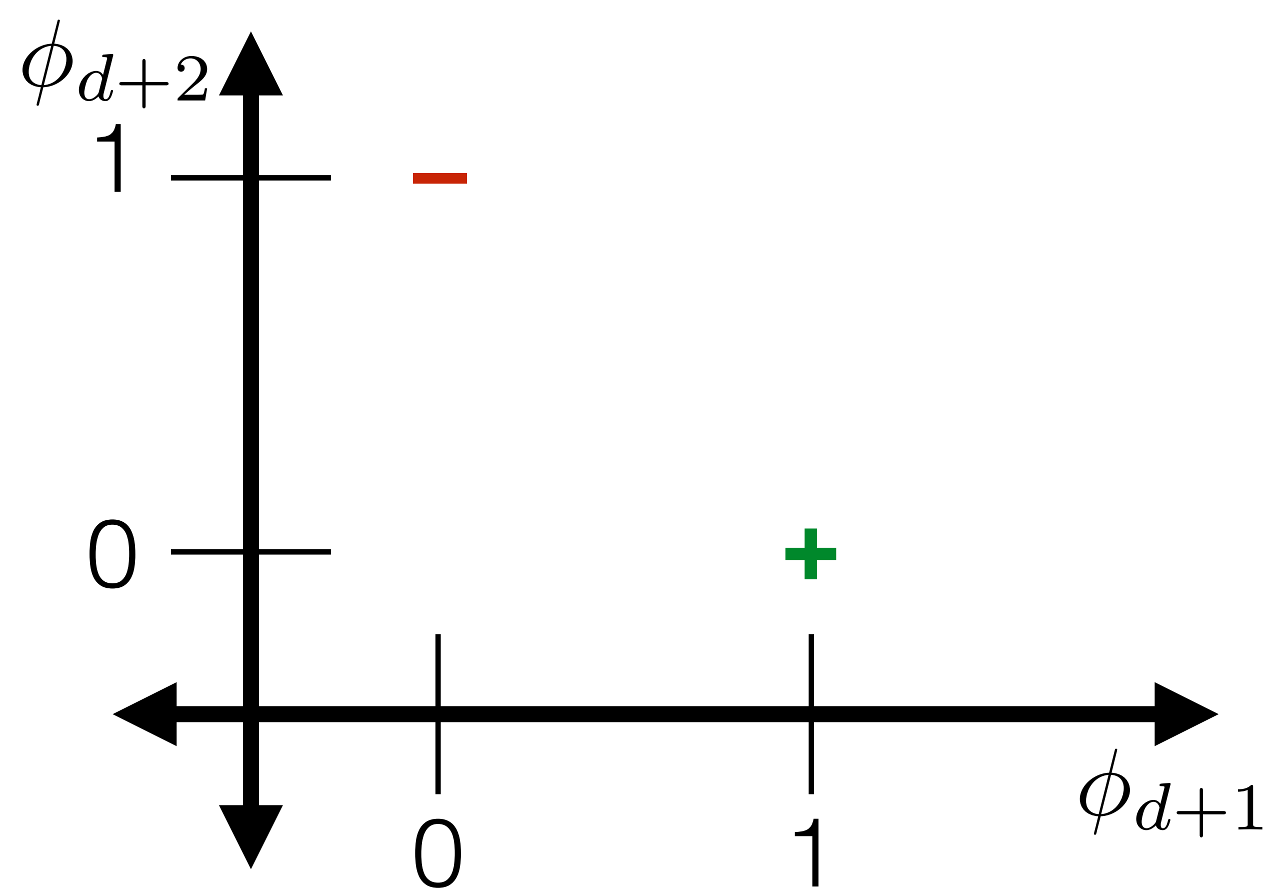


Encode categorical data

- Idea: turn each category into own unique 0-1 feature

	ϕ_d	ϕ_{d+1}	ϕ_{d+2}	ϕ_{d+3}	ϕ_{d+4}
nurse	1	0	0	0	0
admin	0	1	0	0	0
pharmacist	0	0	1	0	0
doctor	0	0	0	1	0
social worker	0	0	0	0	1

- "one-hot encoding"



Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	job	medicines	age	family income (USD)
1	55	0	nurse	pain	40s	133000
2	71	0	admin	beta blockers, pain	20s	34000
3	89	1	nurse	beta blockers	50s	40000
4	67	0	doctor	none	50s	120000

Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	medicines	age	family income (USD)
1	55	0	1,0,0,0,0	pain	40s	133000
2	71	0	0,1,0,0,0	beta blockers, pain	20s	34000
3	89	1	1,0,0,0,0	beta blockers	50s	40000
4	67	0	0,0,0,1,0	none	50s	120000

Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	medicines	age	family income (USD)
1	55	0	1,0,0,0,0	pain	40s	133000
2	71	0	0,1,0,0,0	beta blockers, pain	20s	34000
3	89	1	1,0,0,0,0	beta blockers	50s	40000
4	67	0	0,0,0,1,0	none	50s	120000

Encode categorical data

pain
pain & beta blockers
beta blockers
no medications

Encode categorical data

- Should we use one-hot encoding?

pain
pain & beta blockers
beta blockers
no medications

Encode categorical data

- Should we use one-hot encoding?

	ϕ_d	ϕ_{d+1}	ϕ_{d+2}	ϕ_{d+3}
pain	1	0	0	0
pain & beta blockers	0	1	0	0
beta blockers	0	0	1	0
no medications	0	0	0	1

Encode categorical data

- Should we use one-hot encoding?

	ϕ_d	ϕ_{d+1}	ϕ_{d+2}	ϕ_{d+3}
pain	1	0	0	0
pain & beta blockers	0	1	0	0
beta blockers	0	0	1	0
no medications	0	0	0	1

- Idea: factored encoding

Encode categorical data

- Should we use one-hot encoding?

	ϕ_d	ϕ_{d+1}	ϕ_{d+2}	ϕ_{d+3}
pain	1	0	0	0
pain & beta blockers	0	1	0	0
beta blockers	0	0	1	0
no medications	0	0	0	1

- Idea: factored encoding

	ϕ_d	ϕ_{d+1}
pain	1	0
pain & beta blockers	1	1
beta blockers	0	1
no medications	0	0

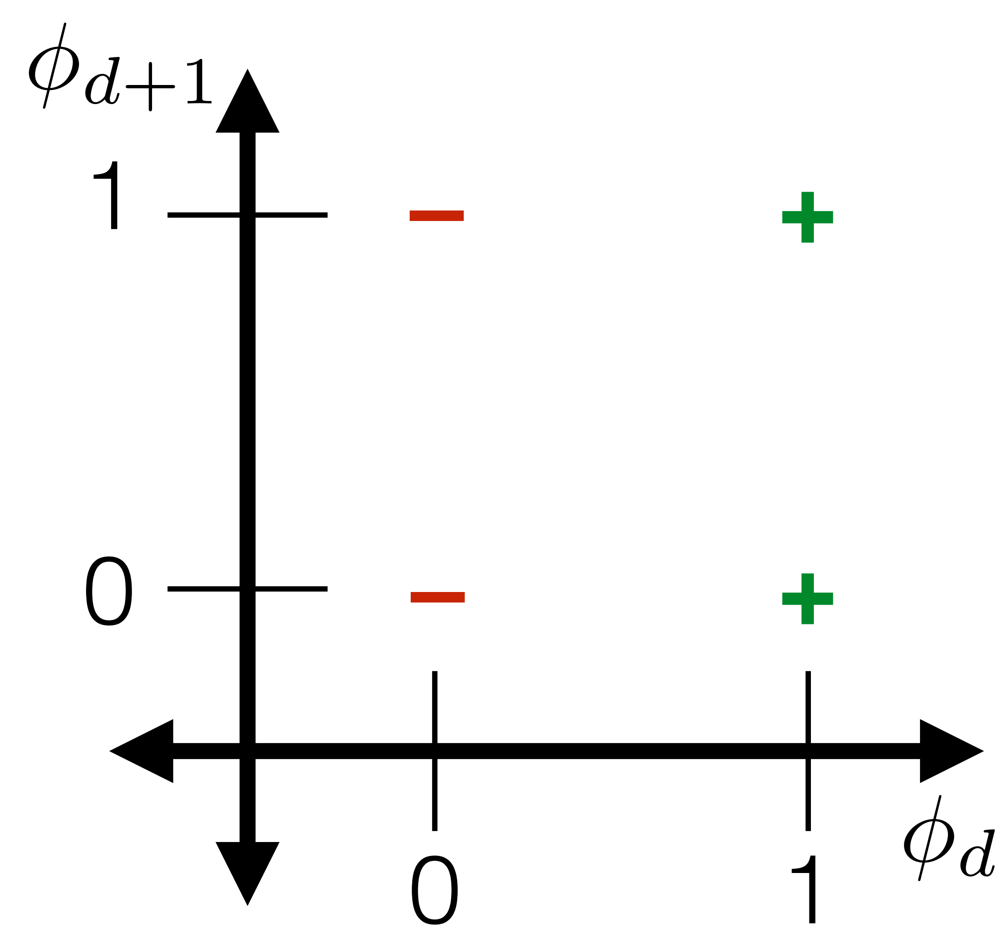
Encode categorical data

- Should we use one-hot encoding?

	ϕ_d	ϕ_{d+1}	ϕ_{d+2}	ϕ_{d+3}
pain	1	0	0	0
pain & beta blockers	0	1	0	0
beta blockers	0	0	1	0
no medications	0	0	0	1

- Idea: factored encoding

	ϕ_d	ϕ_{d+1}
pain	1	0
pain & beta blockers	1	1
beta blockers	0	1
no medications	0	0



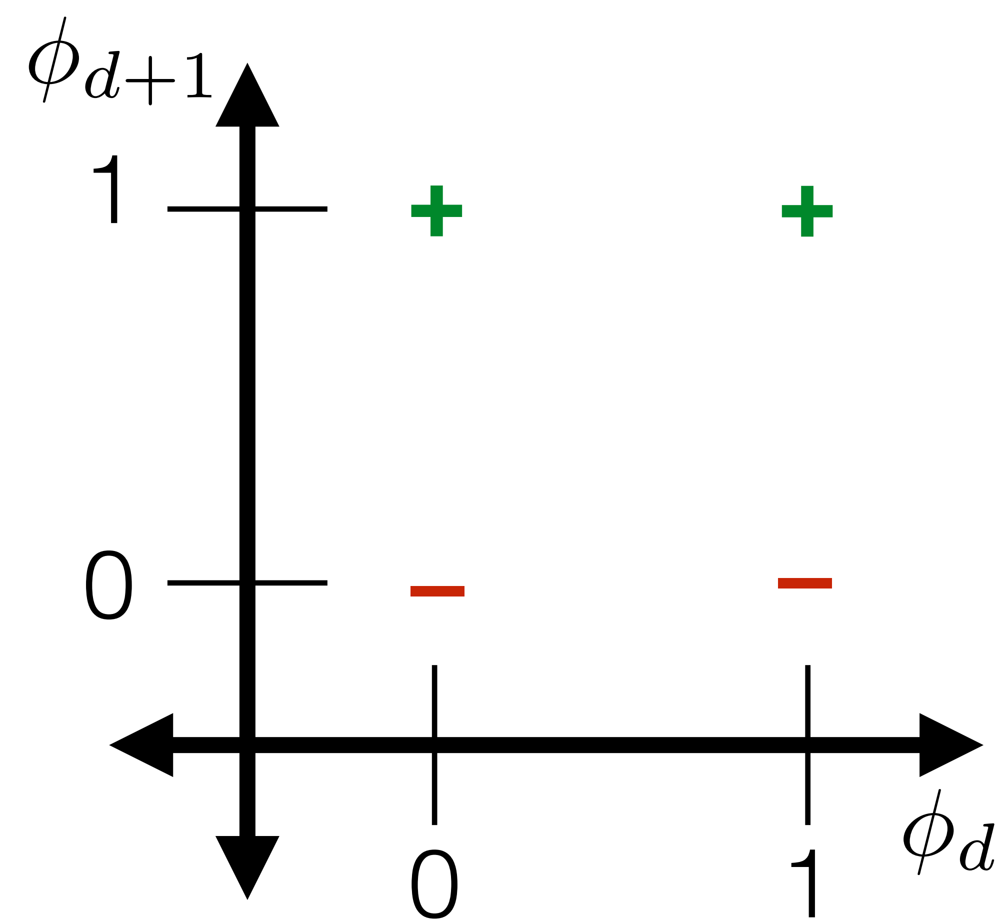
Encode categorical data

- Should we use one-hot encoding?

	ϕ_d	ϕ_{d+1}	ϕ_{d+2}	ϕ_{d+3}
pain	1	0	0	0
pain & beta blockers	0	1	0	0
beta blockers	0	0	1	0
no medications	0	0	0	1

- Idea: factored encoding

	ϕ_d	ϕ_{d+1}
pain	1	0
pain & beta blockers	1	1
beta blockers	0	1
no medications	0	0



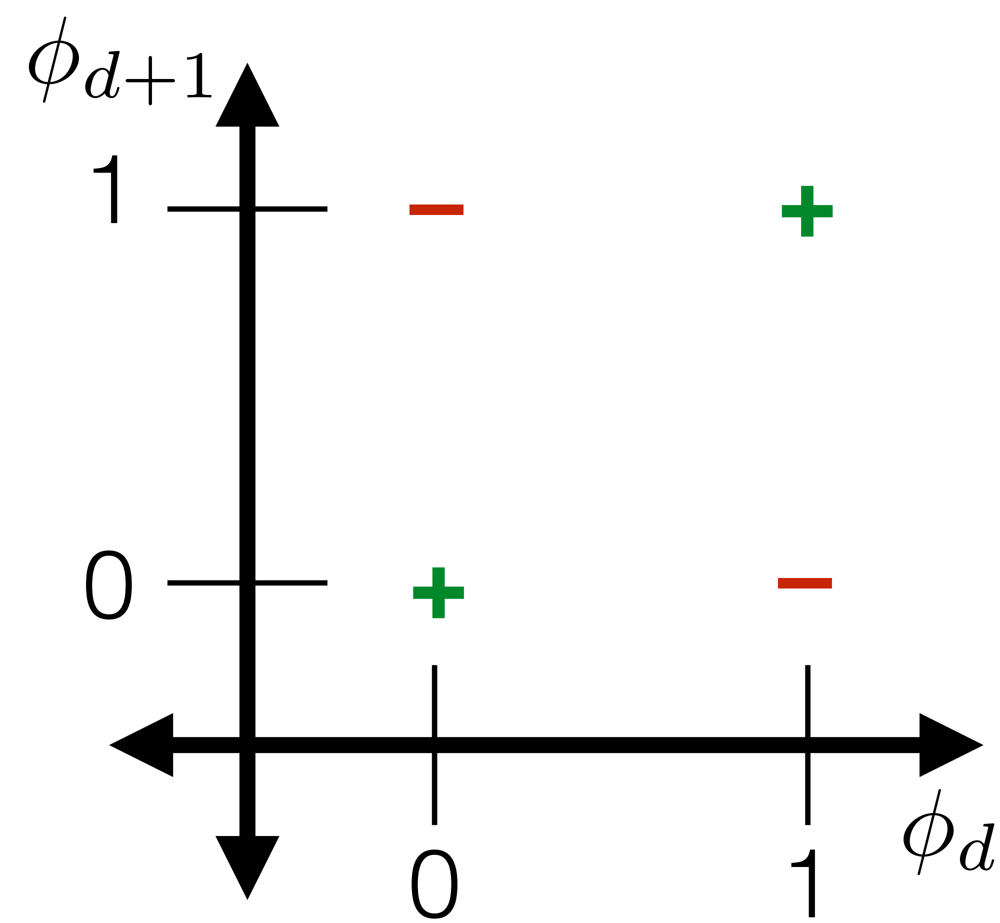
Encode categorical data

- Should we use one-hot encoding?

	ϕ_d	ϕ_{d+1}	ϕ_{d+2}	ϕ_{d+3}
pain	1	0	0	0
pain & beta blockers	0	1	0	0
beta blockers	0	0	1	0
no medications	0	0	0	1

- Idea: factored encoding

	ϕ_d	ϕ_{d+1}
pain	1	0
pain & beta blockers	1	1
beta blockers	0	1
no medications	0	0



Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	medicines	age	family income (USD)
1	55	0	1,0,0,0,0	pain	40s	133000
2	71	0	0,1,0,0,0	beta blockers, pain	20s	34000
3	89	1	1,0,0,0,0	beta blockers	50s	40000
4	67	0	0,0,0,1,0	none	50s	120000

Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	age	family income (USD)
1	55	0	1,0,0,0,0	1,0	40s	133000
2	71	0	0,1,0,0,0	1,1	20s	34000
3	89	1	1,0,0,0,0	0,1	50s	40000
4	67	0	0,0,0,1,0	0,0	50s	120000

Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	age	family income (USD)
1	55	0	1,0,0,0,0	1,0	40s	133000
2	71	0	0,1,0,0,0	1,1	20s	34000
3	89	1	1,0,0,0,0	0,1	50s	40000
4	67	0	0,0,0,1,0	0,0	50s	120000

Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	age	family income (USD)
1	55	0	1,0,0,0,0	1,0	45	133000
2	71	0	0,1,0,0,0	1,1	25	34000
3	89	1	1,0,0,0,0	0,1	55	40000
4	67	0	0,0,0,1,0	0,0	55	120000

Using a representative # for a range

age
45
25
55
55

Using a representative # for a range

- Potential pitfall: level of detail might be treated as meaningful (by you or others using the data)

age
45
25
55
55

Using a representative # for a range

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age
45
25
55
55

[https://fusion.tv/story/287592/internet-mapping-glitch-kansas-farm/?utm_medium=social]

Using a representative # for a range

- Potential pitfall: level of detail might be treated as meaningful (by you or others using the data)
- A way to diagnose many problems: plot your data!

age
45
25
55
55

[https://fusion.tv/story/287592/internet-mapping-glitch-kansas-farm/?utm_medium=social]

Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	age	family income (USD)
1	55	0	1,0,0,0,0	1,0	45	133000
2	71	0	0,1,0,0,0	1,1	25	34000
3	89	1	1,0,0,0,0	0,1	55	40000
4	67	0	0,0,0,1,0	0,0	55	120000

Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	decade	family income (USD)
1	55	0	1,0,0,0,0	1,0	4	133000
2	71	0	0,1,0,0,0	1,1	2	34000
3	89	1	1,0,0,0,0	0,1	5	40000
4	67	0	0,0,0,1,0	0,0	5	120000

Encode ordinal data

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  - E.g. Likert scale:

Strongly disagree	Disagree	Neutral	Agree	Strongly agree
1	2	3	4	5

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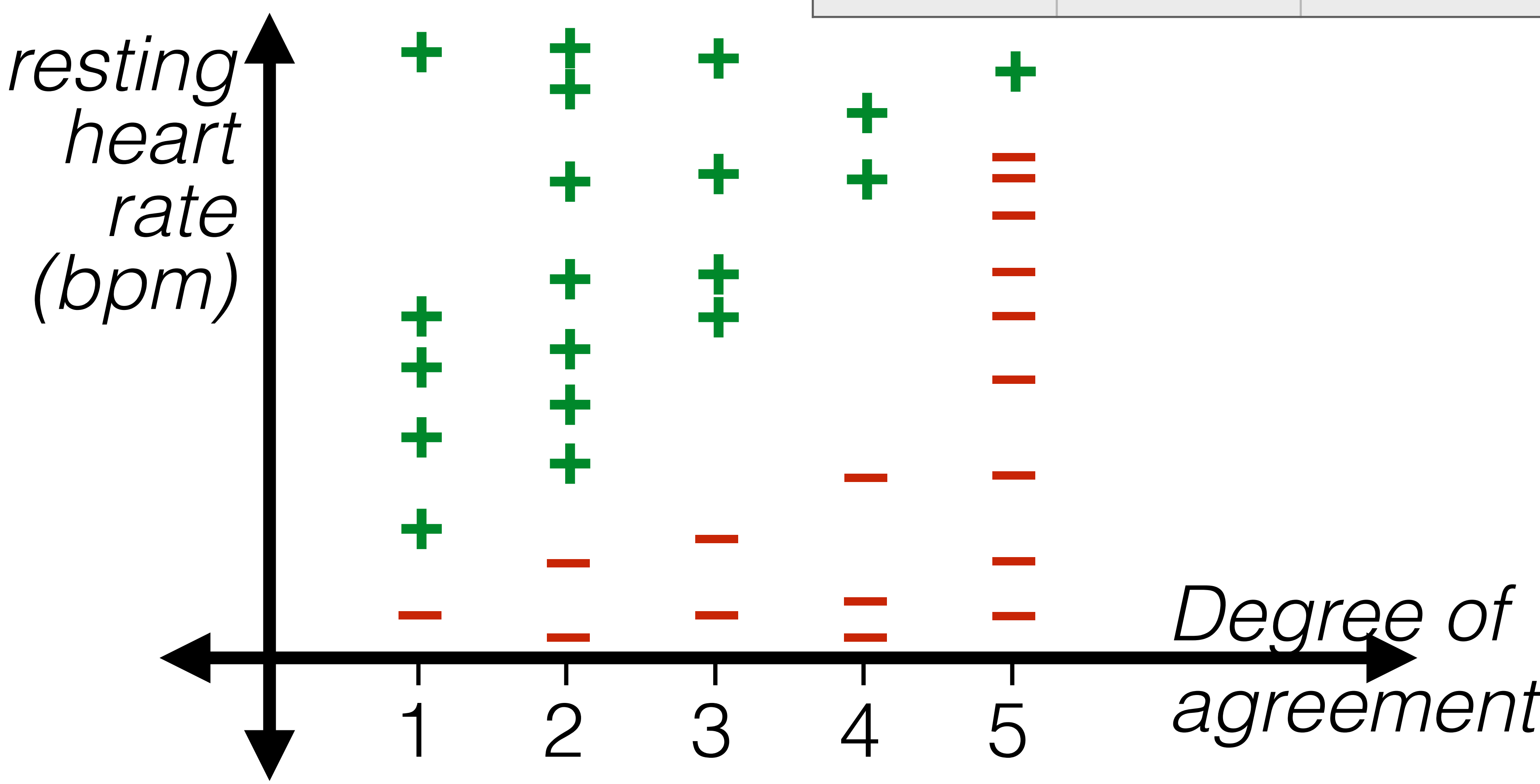

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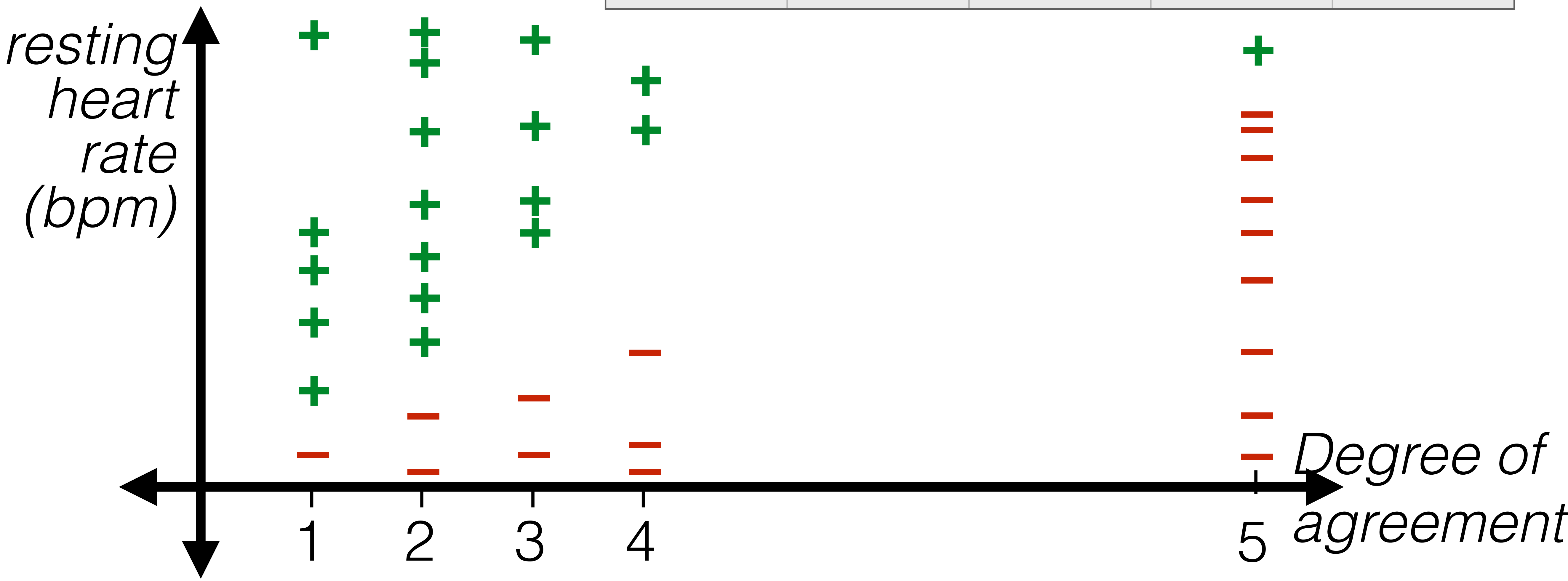

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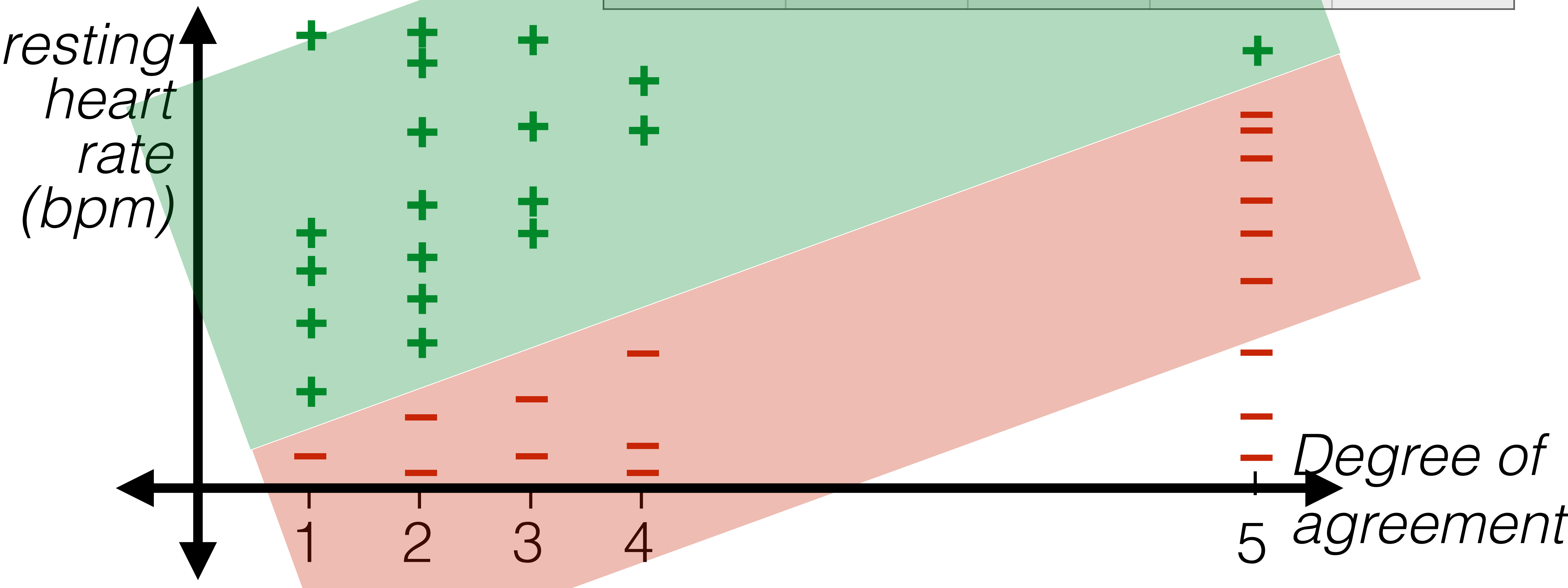

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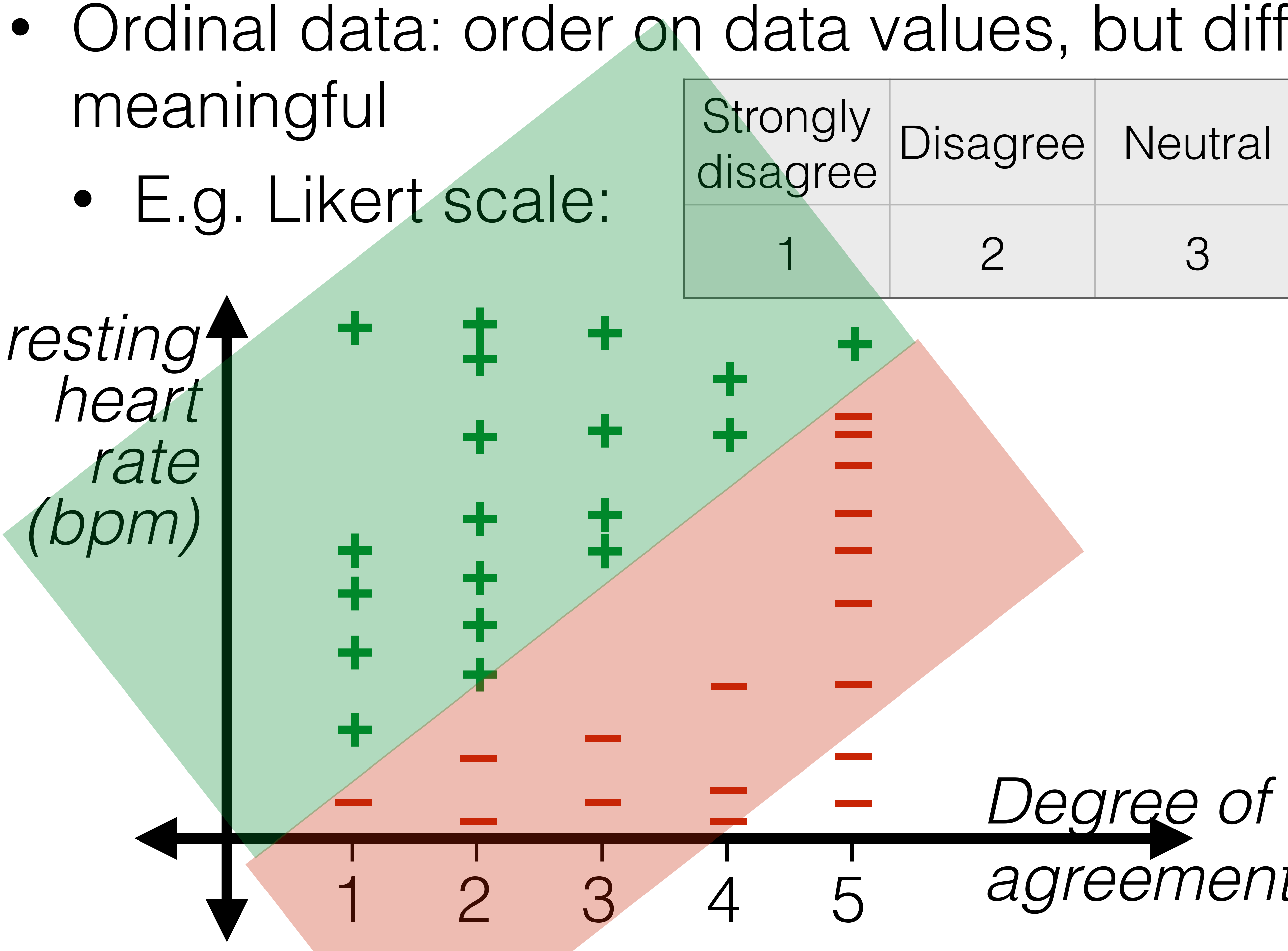

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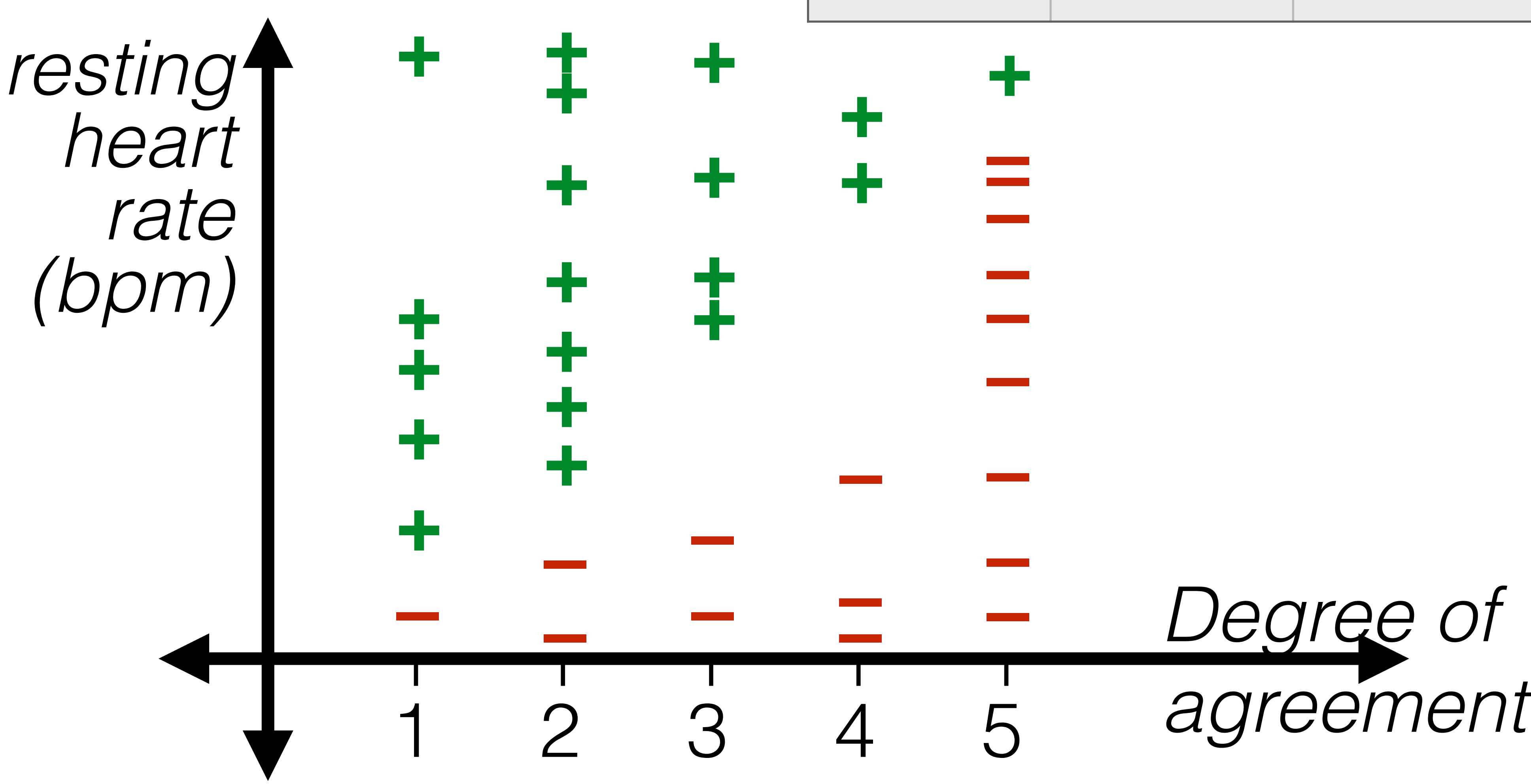

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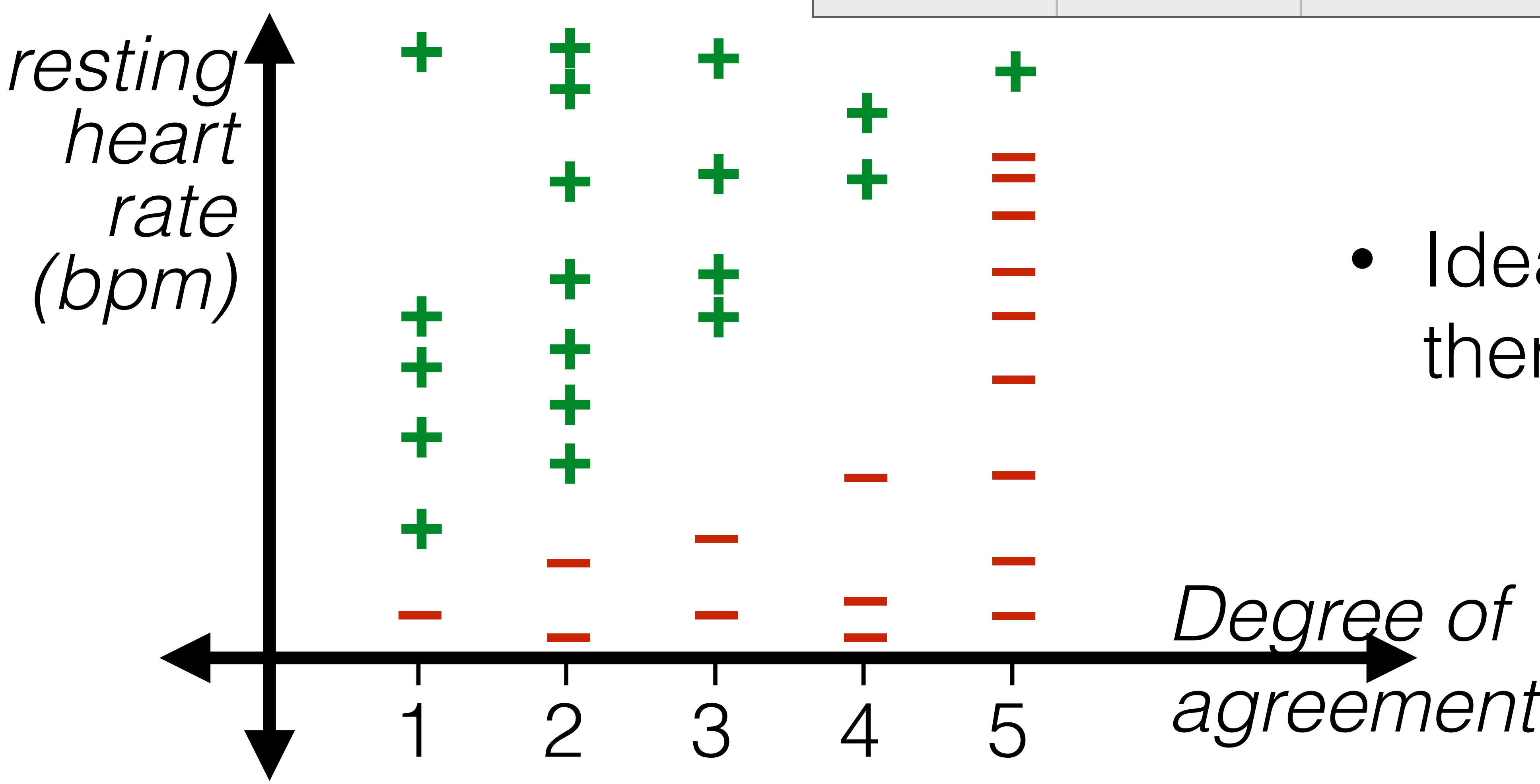
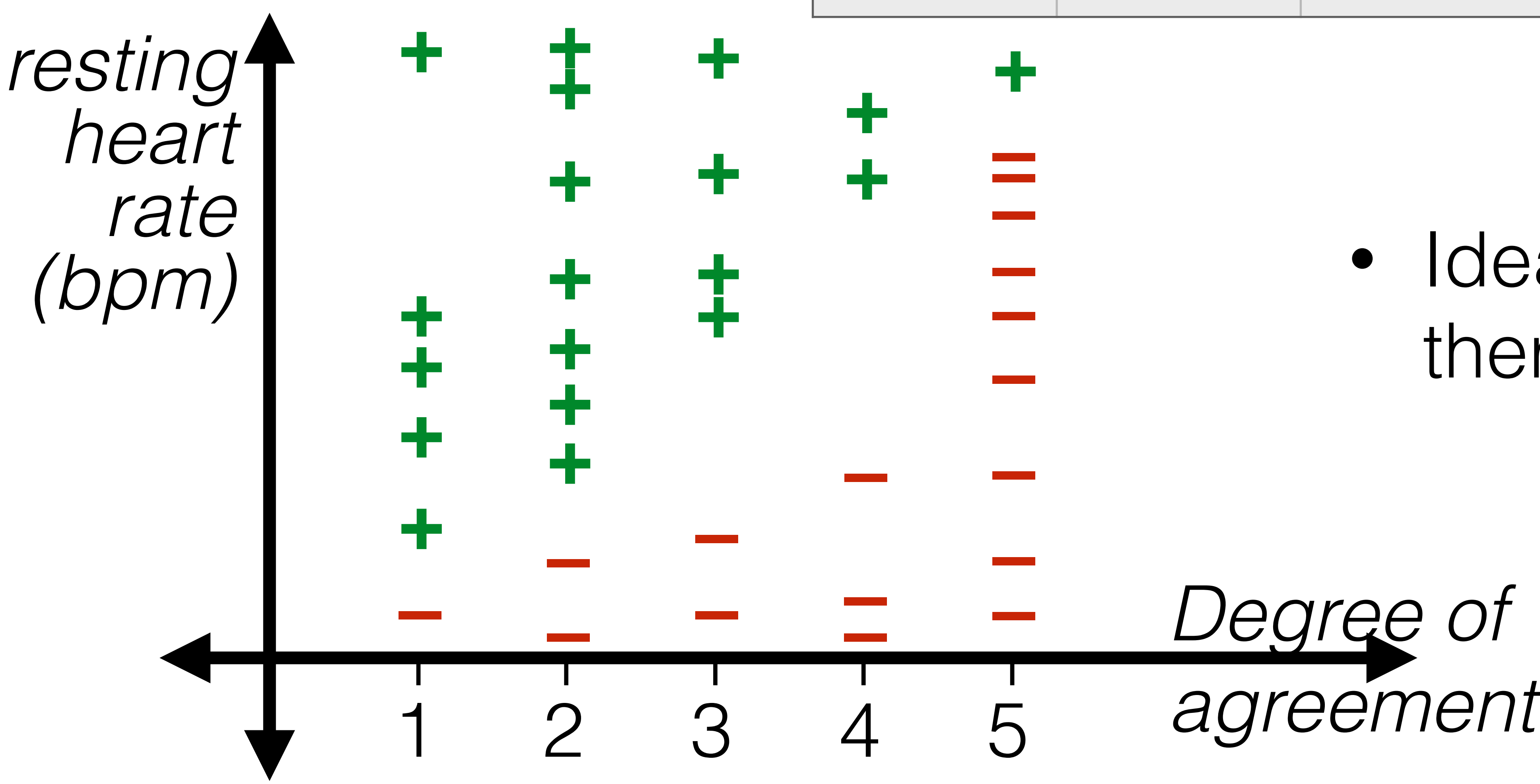


- Idea: Unary/ thermometer code

Encode ordinal data

- Numerical data: order on data values, and differences in value are meaningful
- Categorical data: no order on data values
- Ordinal data: order on data values, but differences not meaningful
  - E.g. Likert scale:

Strongly disagree	Disagree	Neutral	Agree	Strongly agree
1,0,0,0,0	1,1,0,0,0	1,1,1,0,0	1,1,1,1,0	1,1,1,1,1



- Idea: Unary/ thermometer code

Encode data in usable form

- Identify the features and encode as real numbers

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	decade	family income (USD)
1	55	0	1,0,0,0,0	1,0	4	133000
2	71	0	0,1,0,0,0	1,1	2	34000
3	89	1	1,0,0,0,0	0,1	5	40000
4	67	0	0,0,0,1,0	0,0	5	120000

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2	71	0	0,1,0,0,0	1,1	2	34000
3	89	1	1,0,0,0,0	0,1	5	40000
4	67	0	0,0,0,1,0	0,0	5	120000

Encode numerical data

Encode numerical data

- A closer look at the output of a linear classifier

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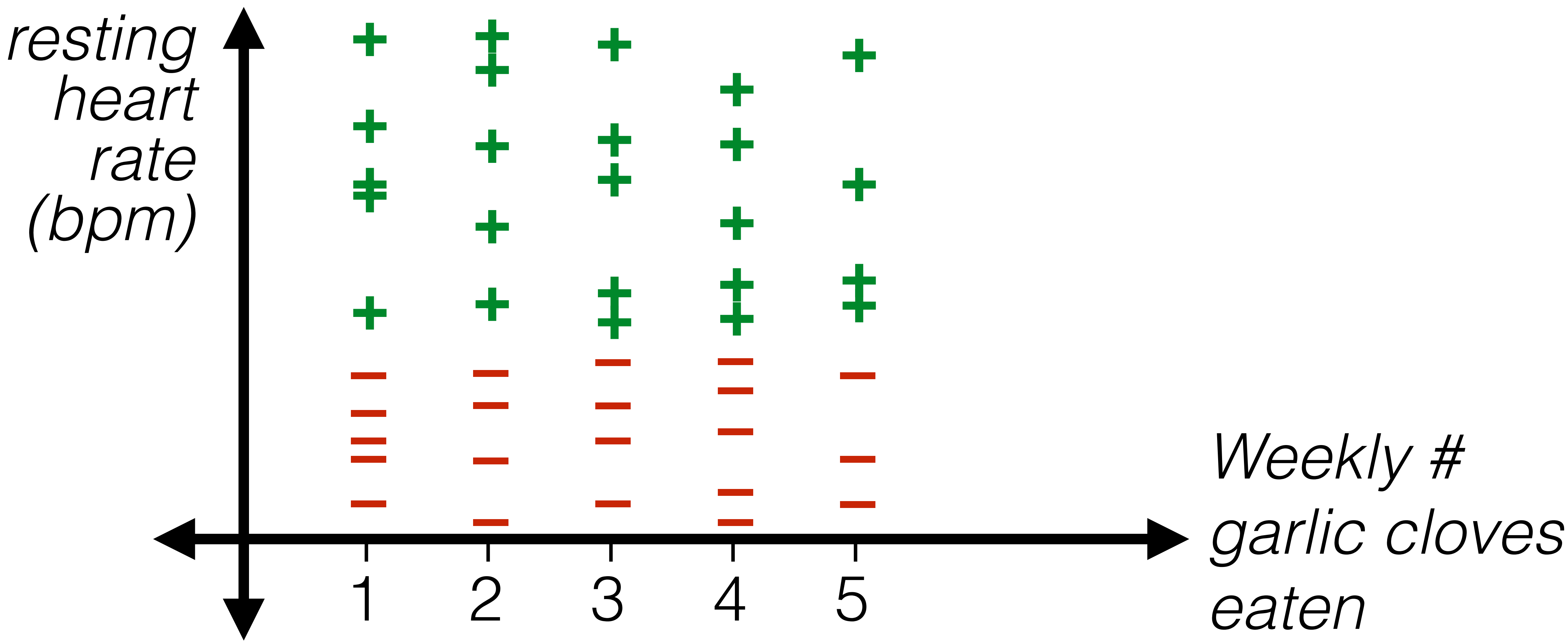

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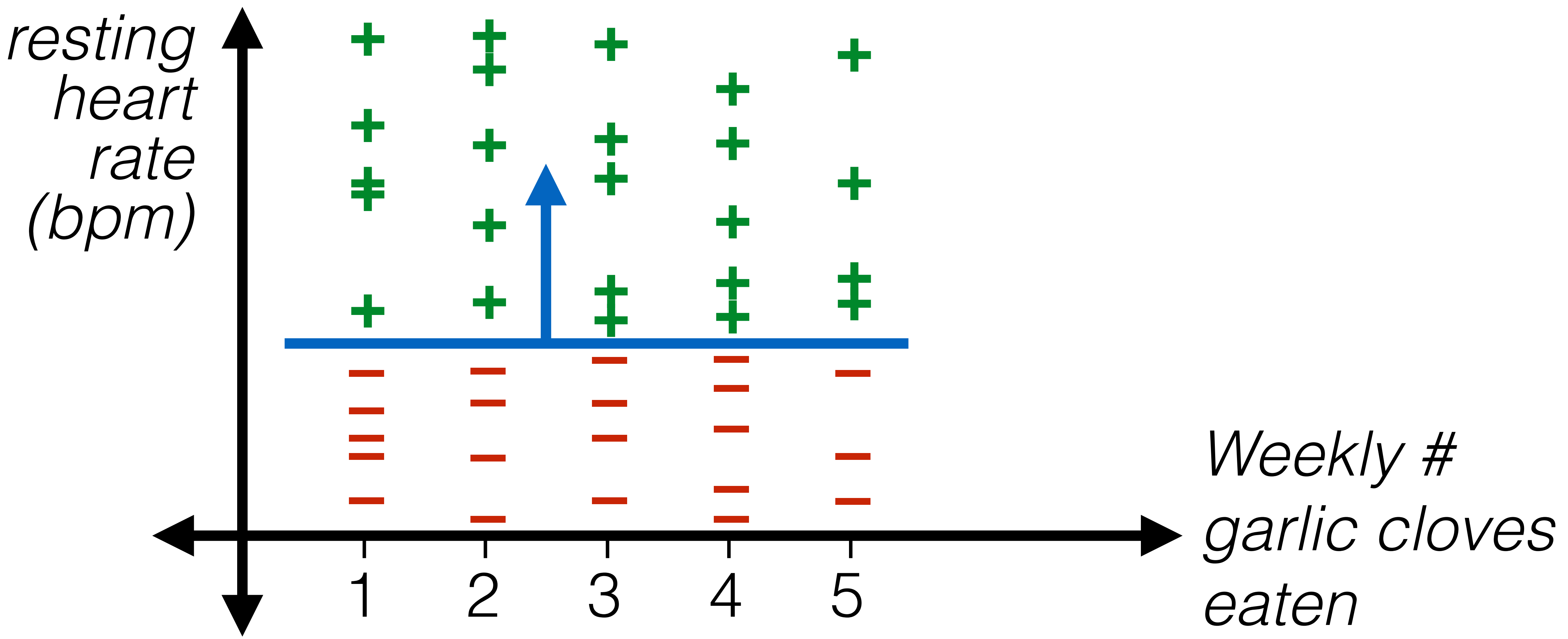

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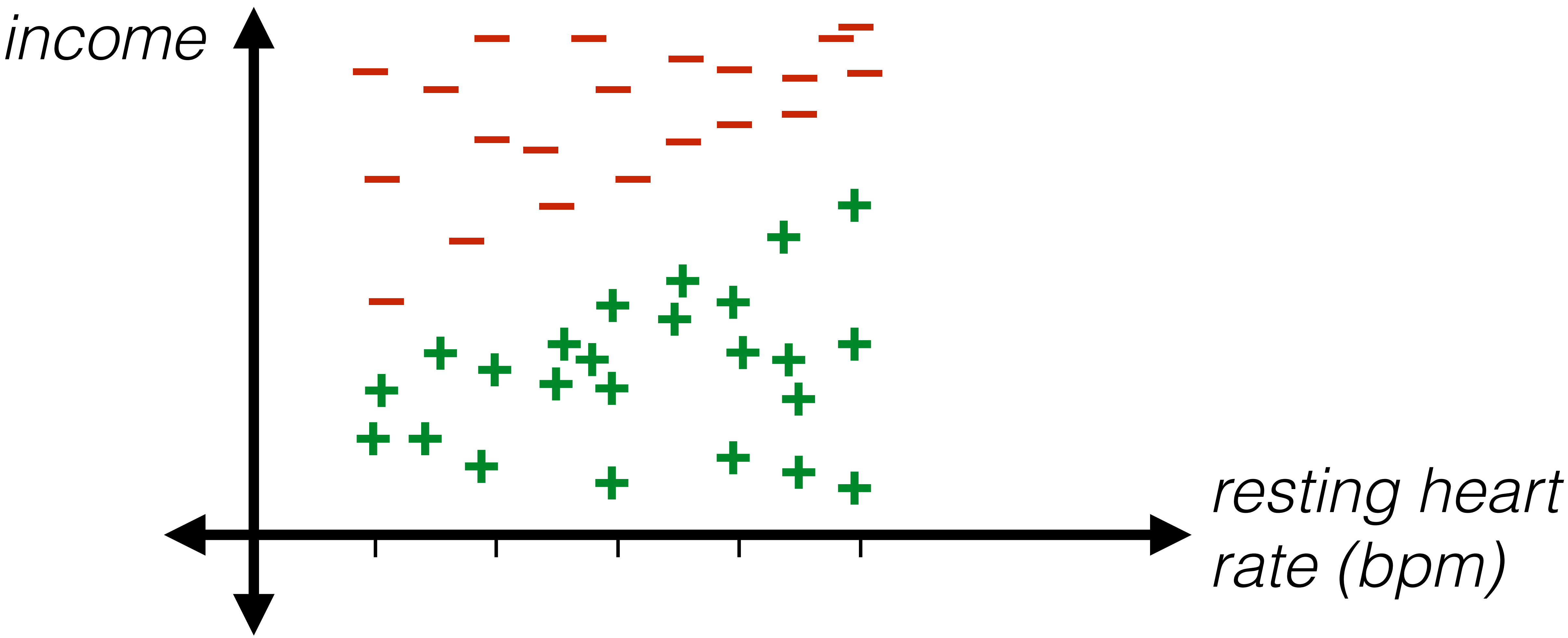

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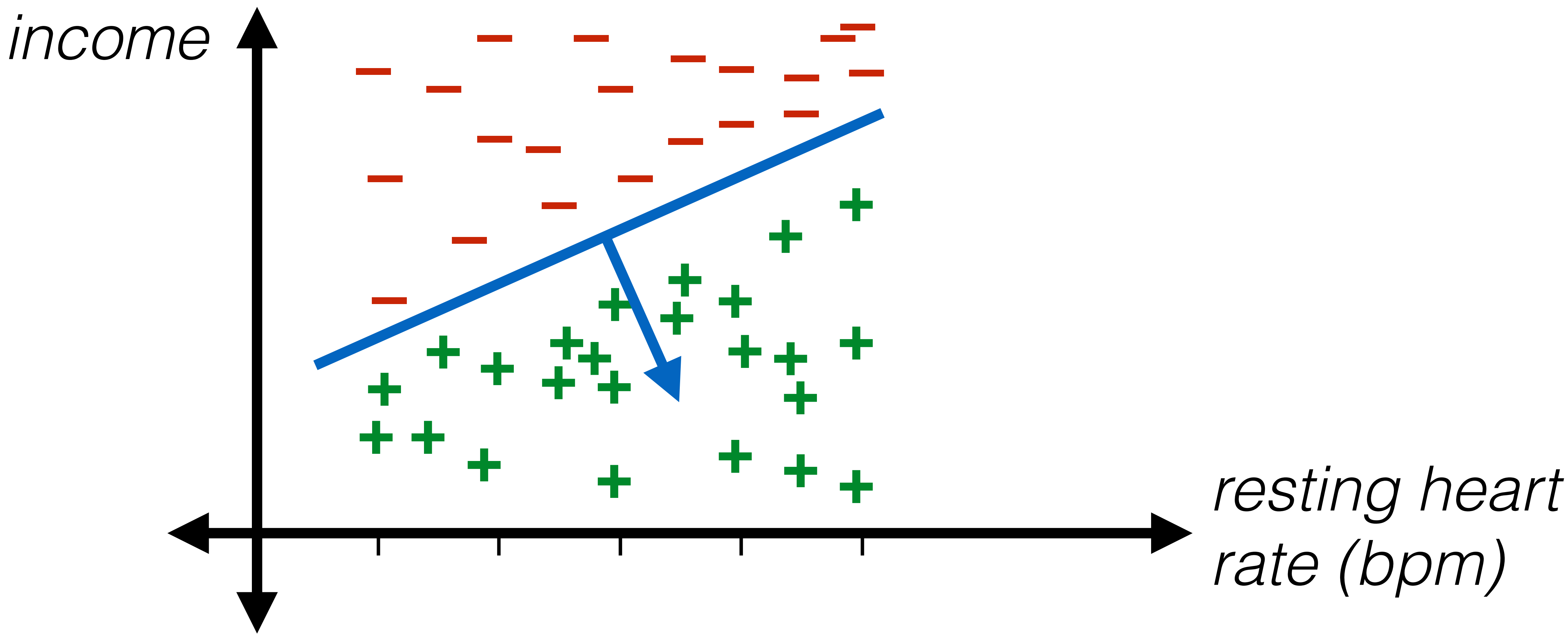

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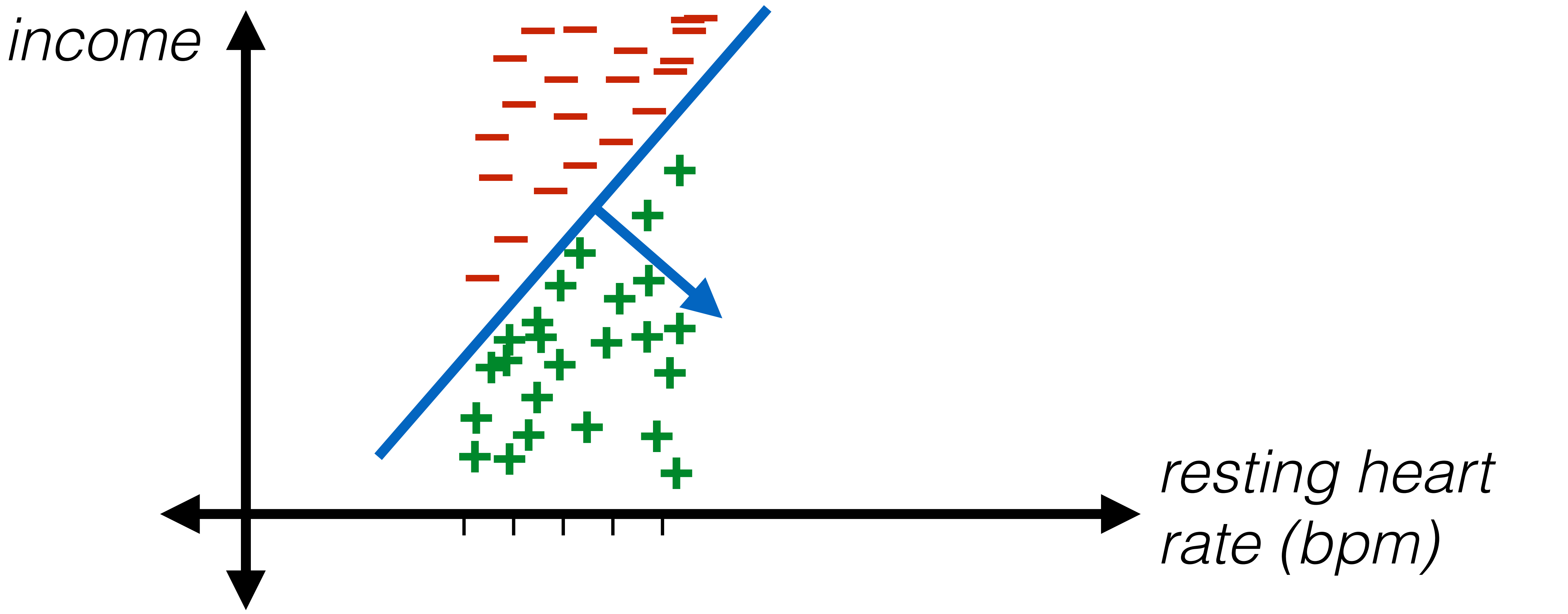

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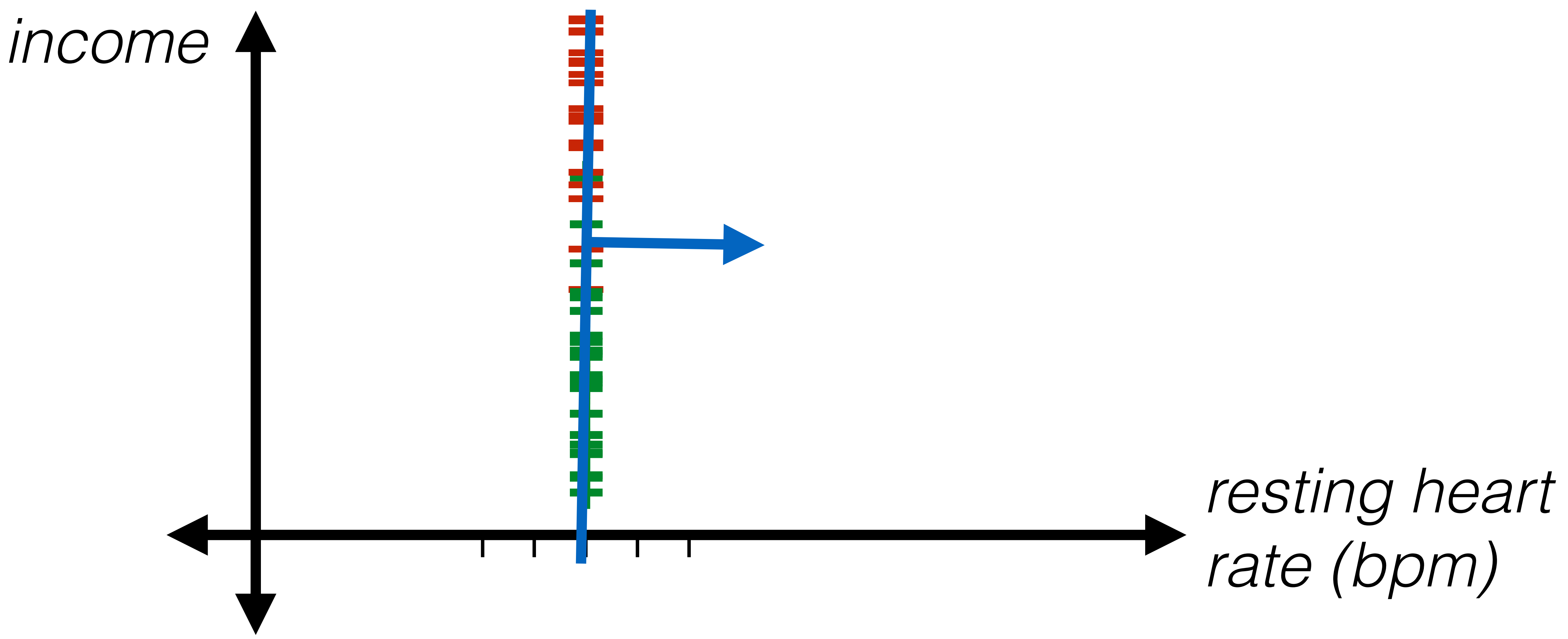
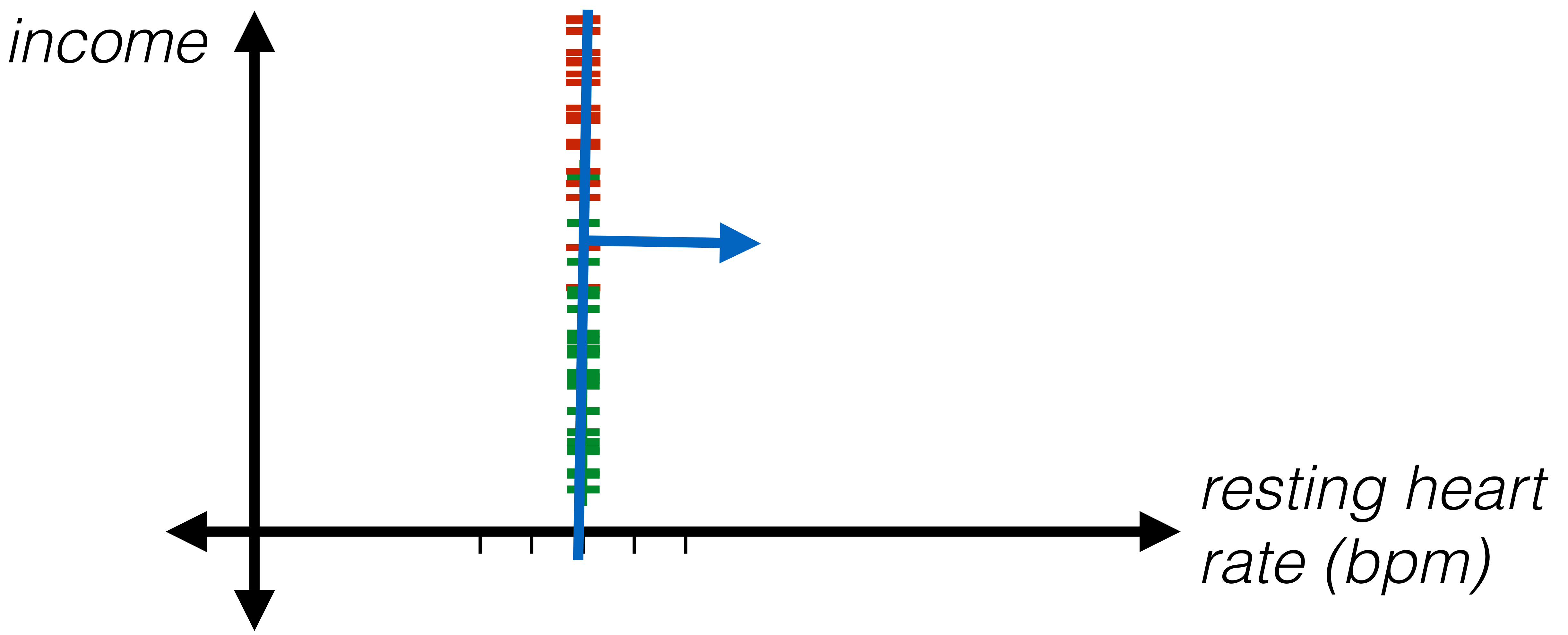


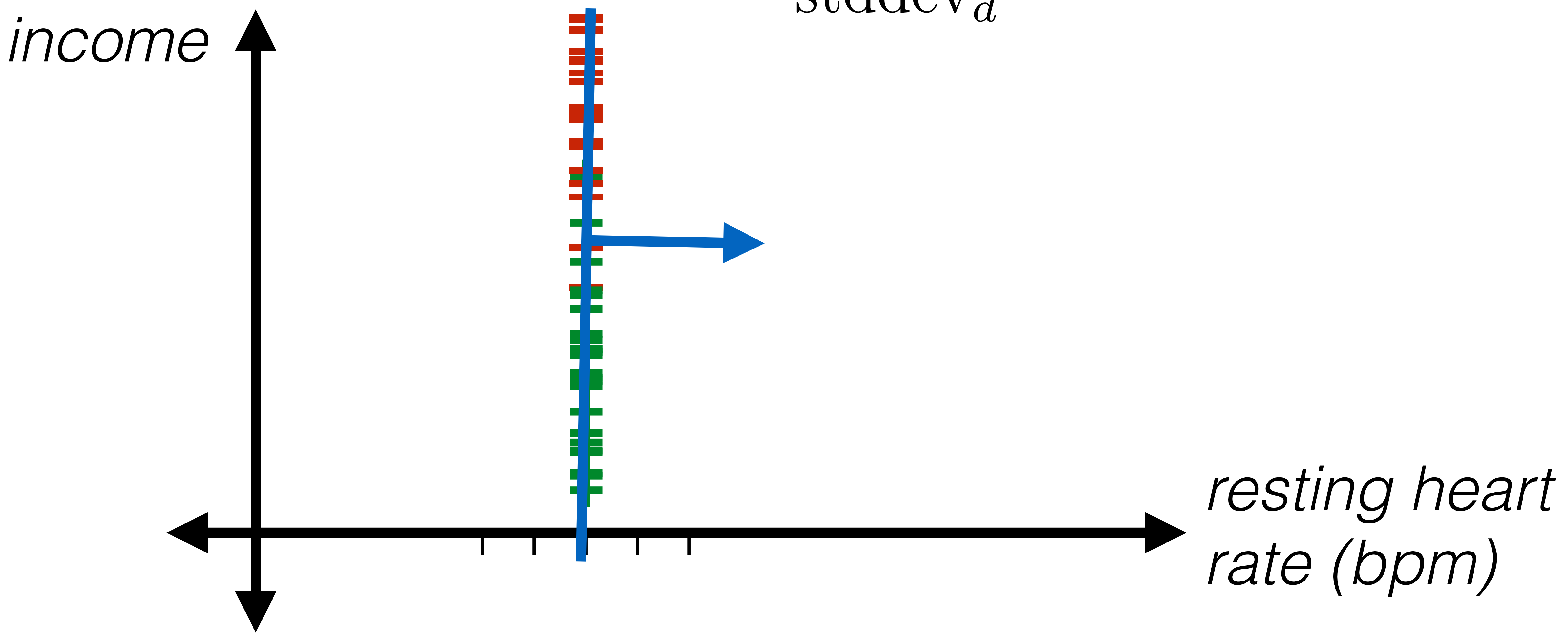
Encode numerical data

- A closer look at the output of a linear classifier
- Idea: standardize numerical data



Encode numerical data

- A closer look at the output of a linear classifier
- Idea: standardize numerical data
    - For *d*th feature: $\phi_d^{(k)} = \dfrac{x_d^{(k)} - \text{mean}_d}{\text{stddev}_d}$



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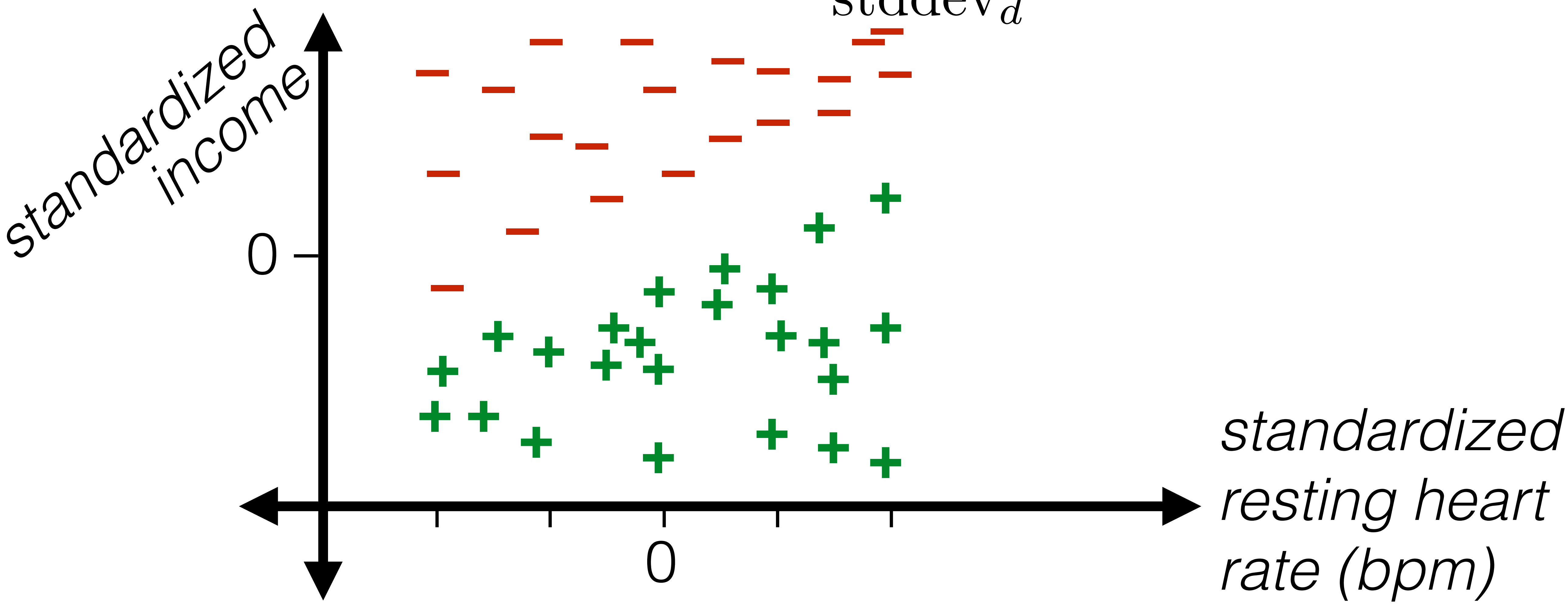

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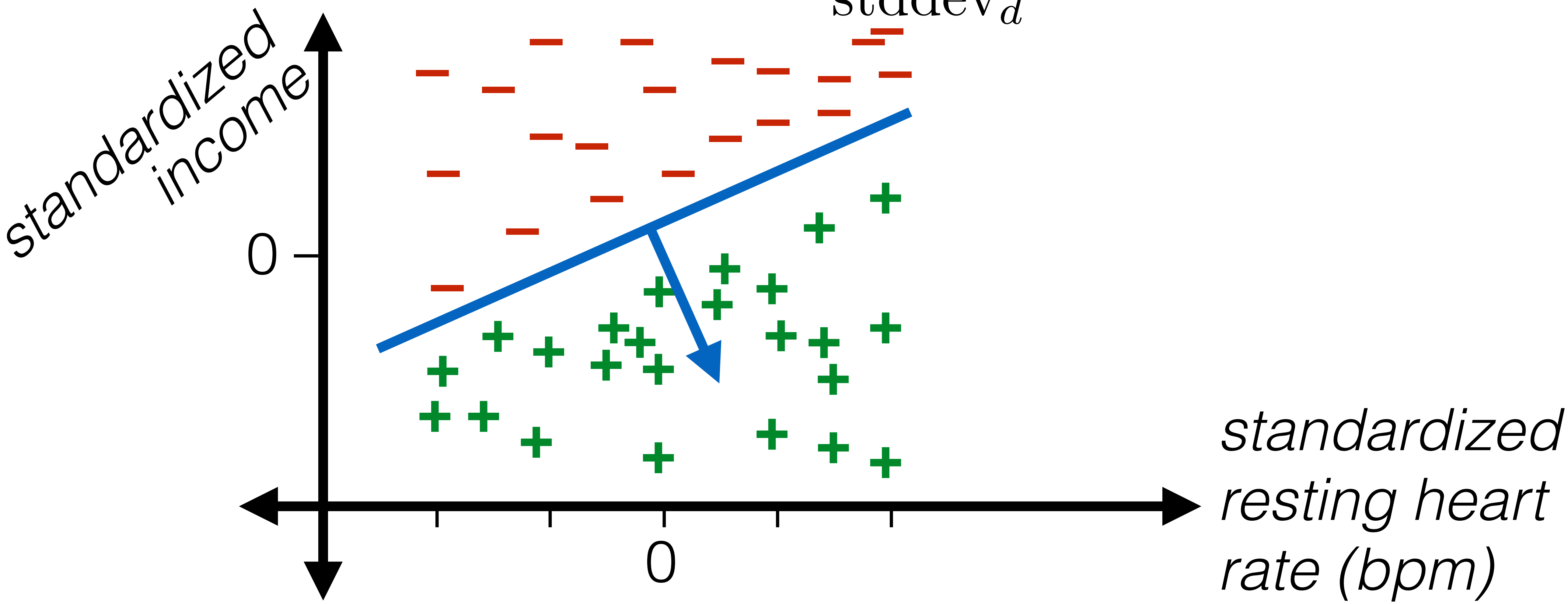

More benefits of plotting your data

More benefits of plotting your data

- And talking to experts

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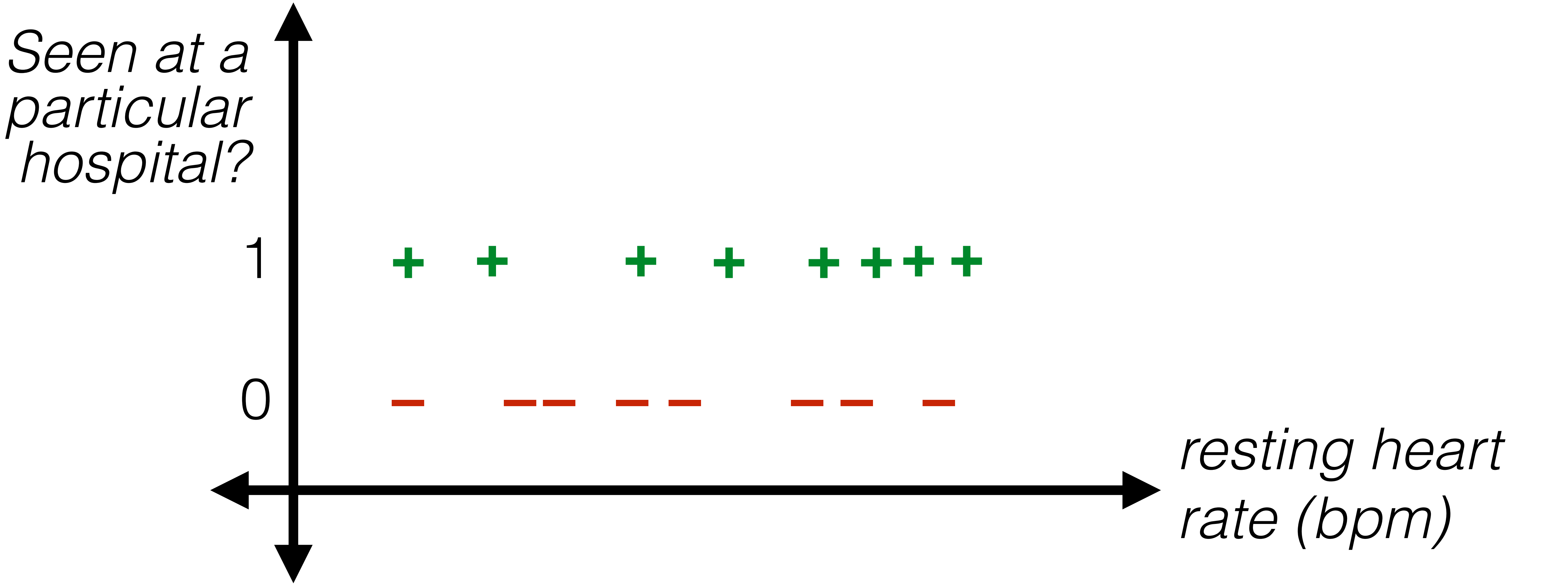

Encode data in usable form

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	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	decade	family income (USD)
1	55	0	1,0,0,0,0	1,0	4	133000
2	71	0	0,1,0,0,0	1,1	2	34000
3	89	1	1,0,0,0,0	0,1	5	40000
4	67	0	0,0,0,1,0	0,0	5	120000

Encode data in usable form

- Identify the features and encode as real numbers
- Standardize numerical features

	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	decade	family income (USD)
1	55	0	1,0,0,0,0	1,0	4	133000
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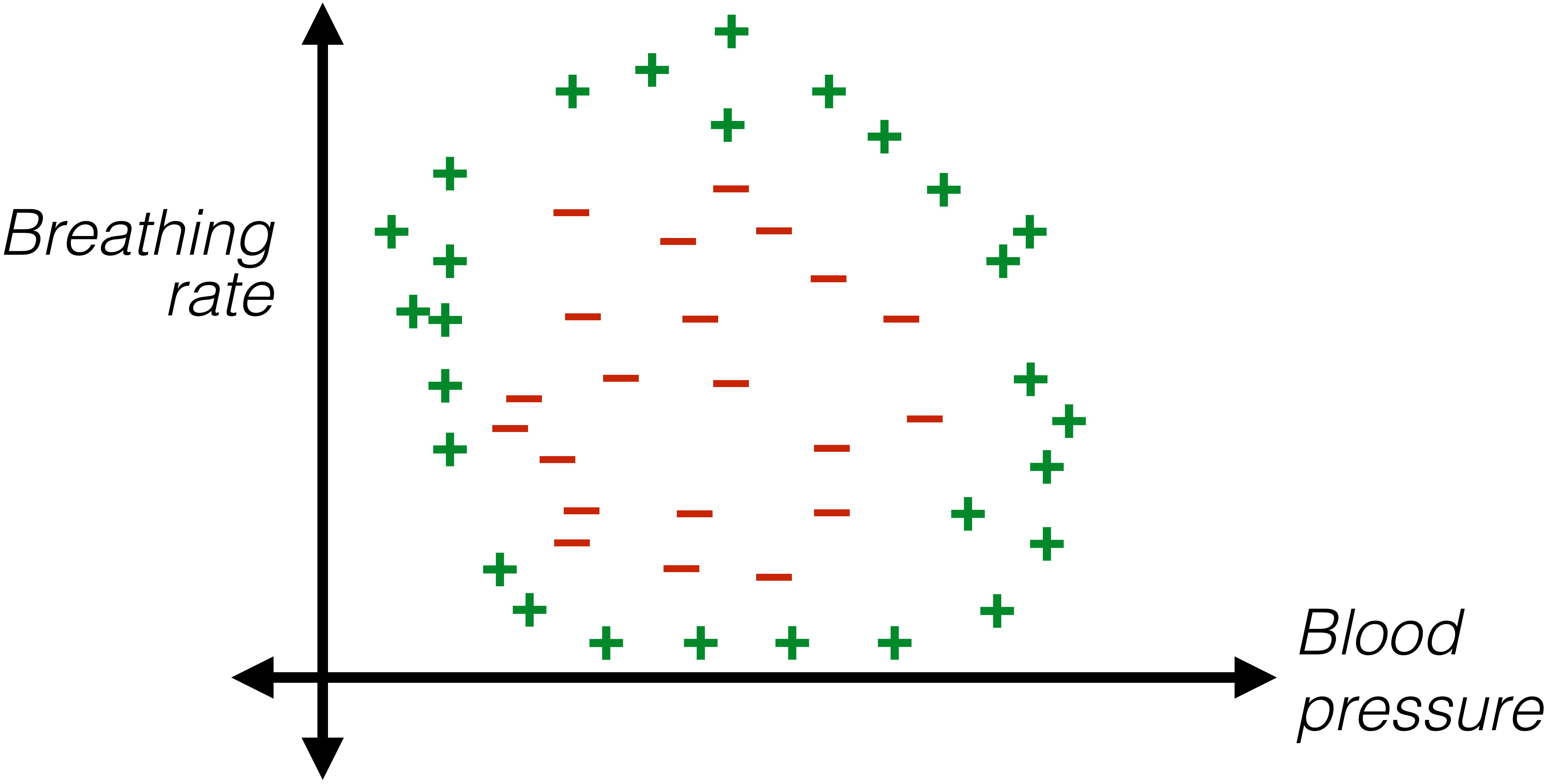
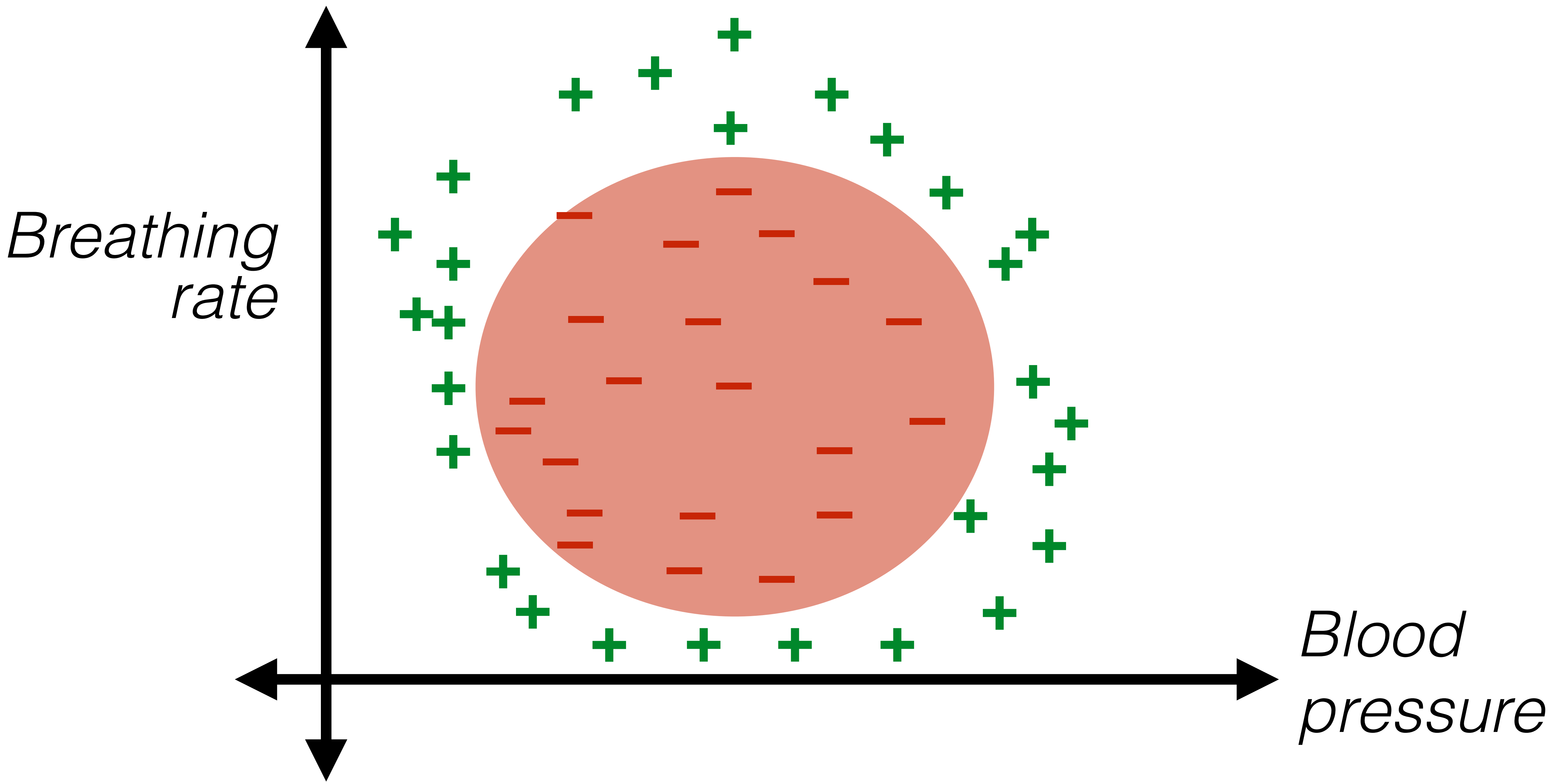
4	67	0	0,0,0,1,0	0,0	5	120000

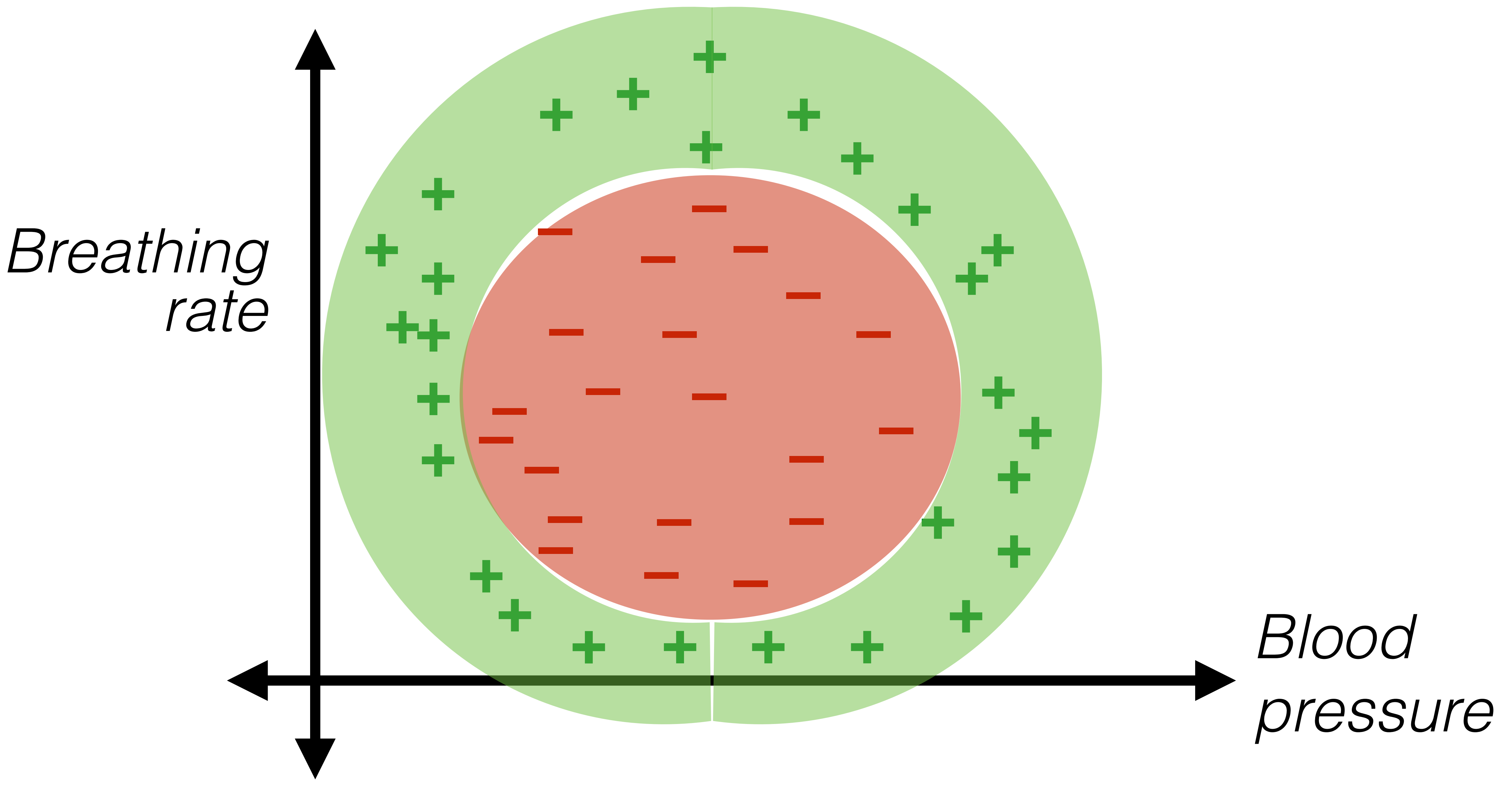
Encode data in usable form

- Identify the features and encode as real numbers
- Standardize numerical features

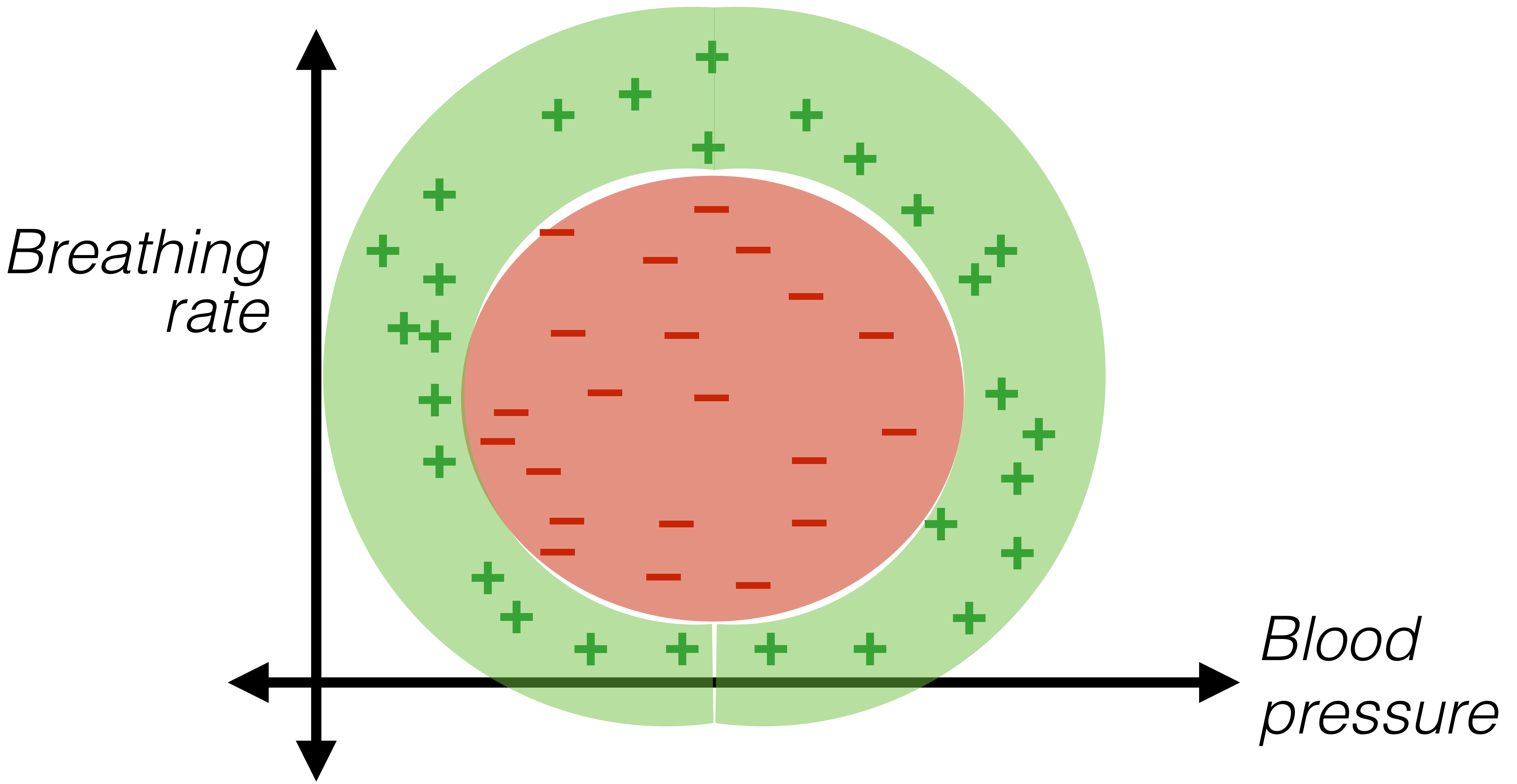
	resting heart rate (bpm)	pain?	j1,j2,j3,j4,j5	m1, m2	decade	family income (USD)
1	-1.5	0	1,0,0,0,0	1,0	1	2.075
2	0.1	0	0,1,0,0,0	1,1	-1	-0.4
3	1.9	1	1,0,0,0,0	0,1	2	-0.25
4	-0.3	0	0,0,0,1,0	0,0	2	1.75


Breathing rate
Blood pressure


Breathing rate
Blood pressure


Breathing rate
Blood pressure

Nonlinear boundaries



Classification boundaries

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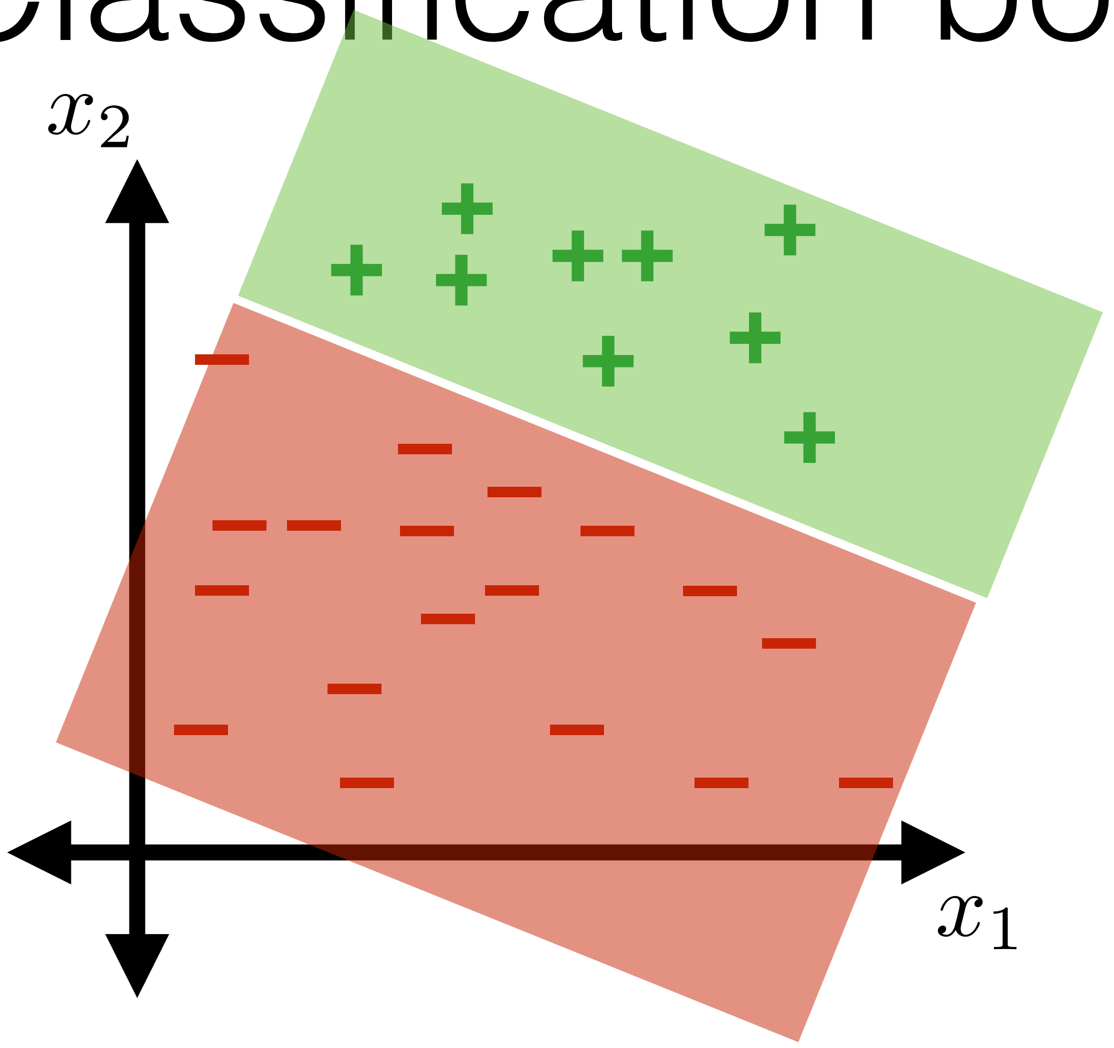

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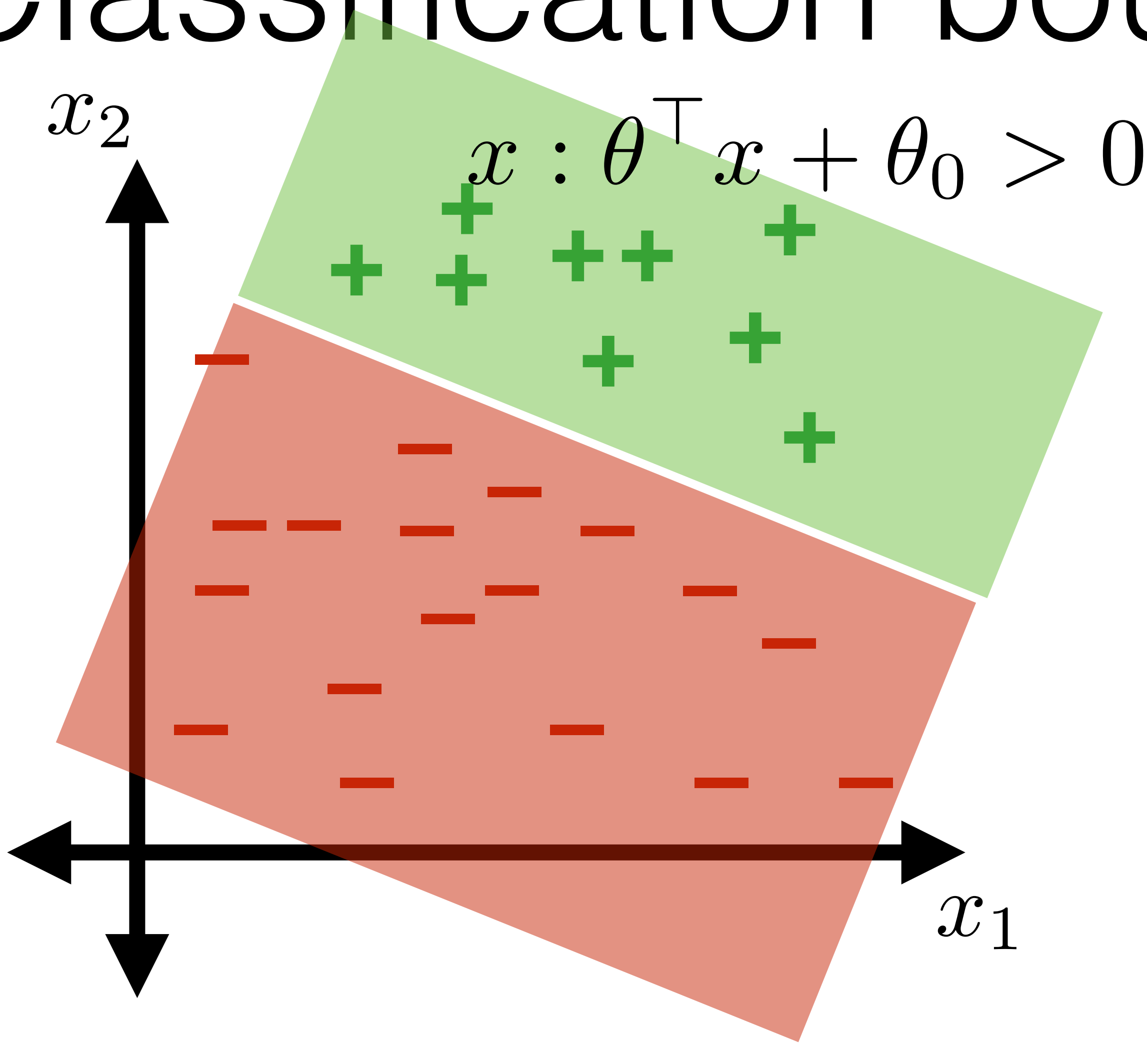

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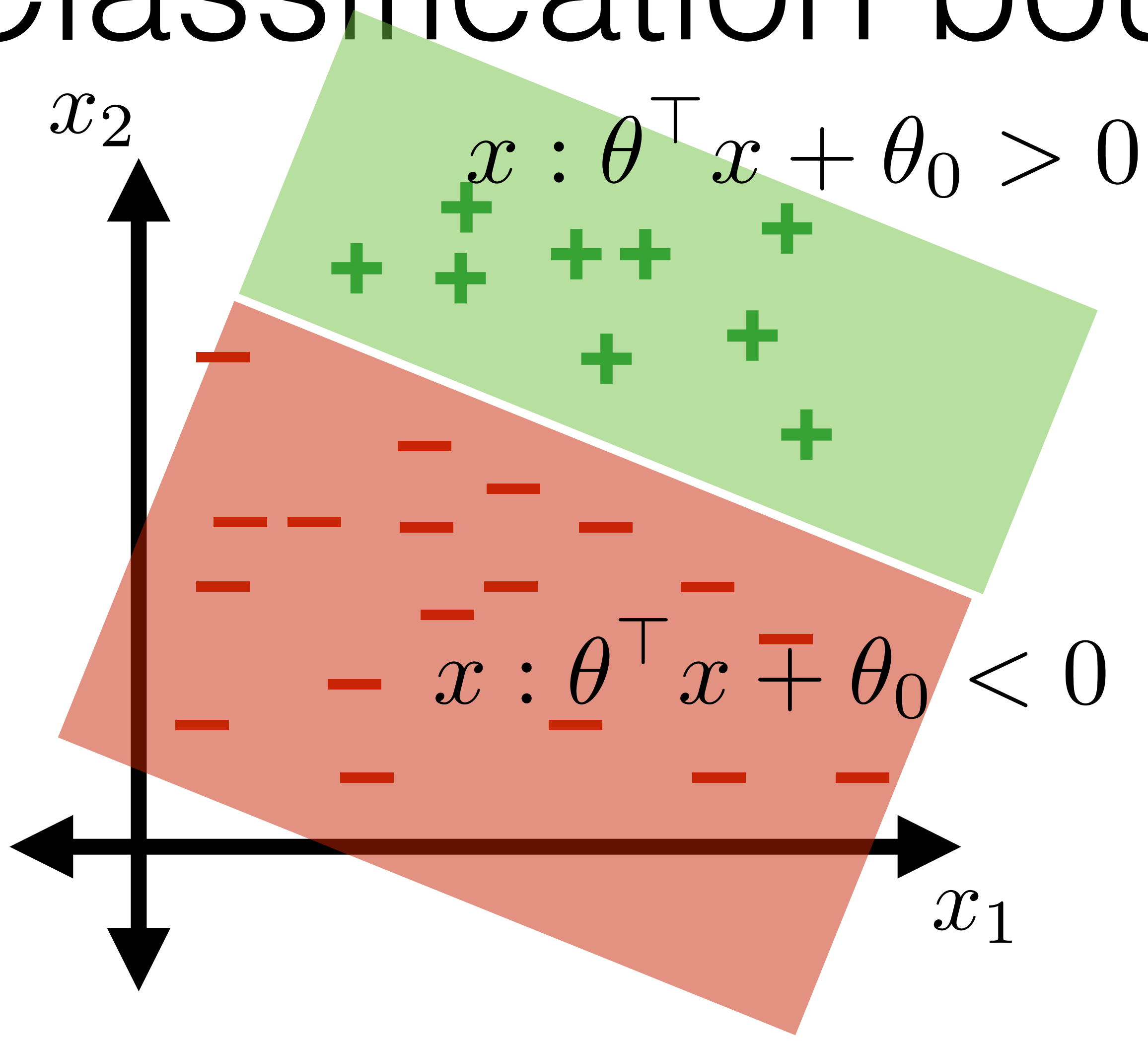

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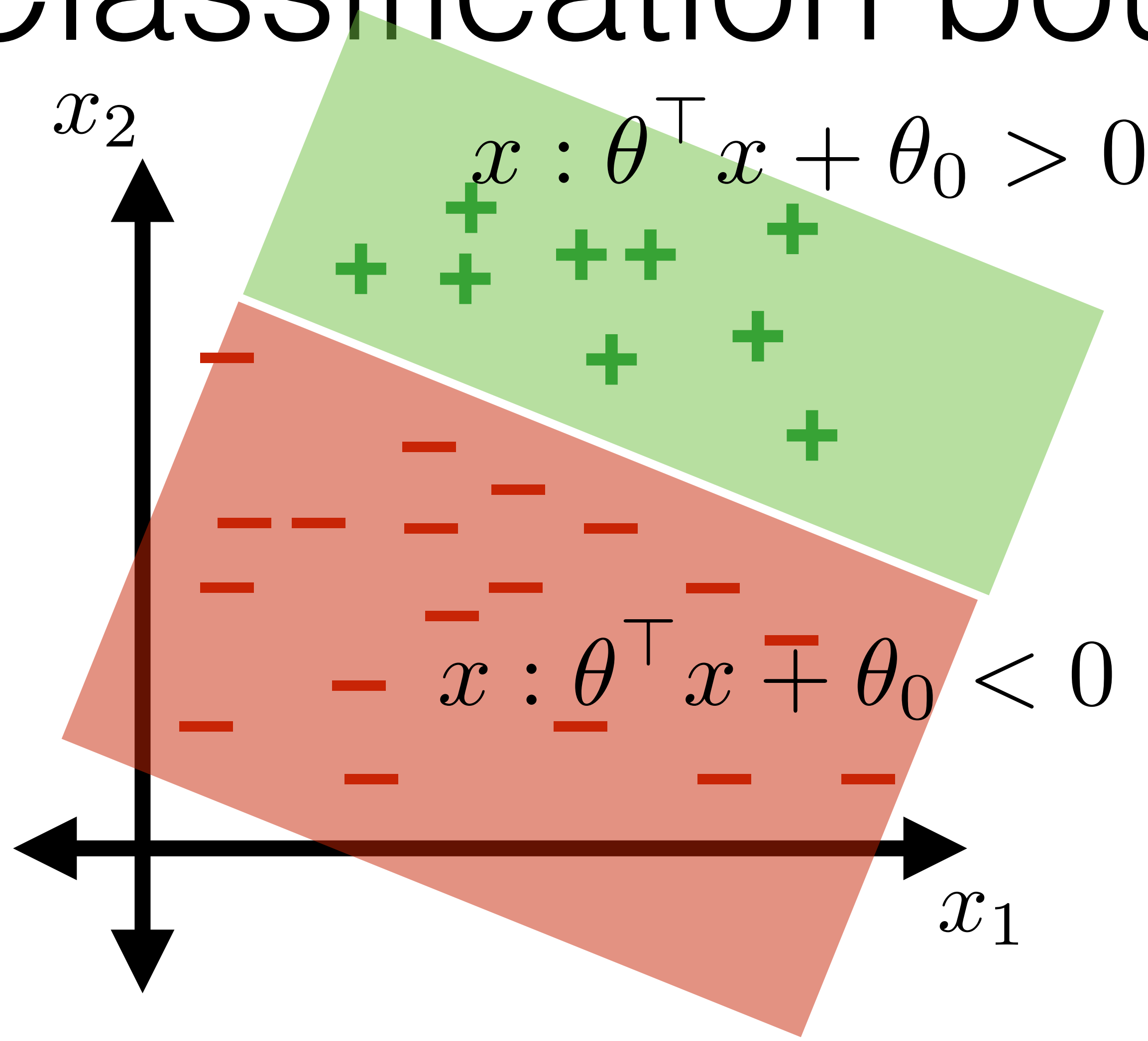

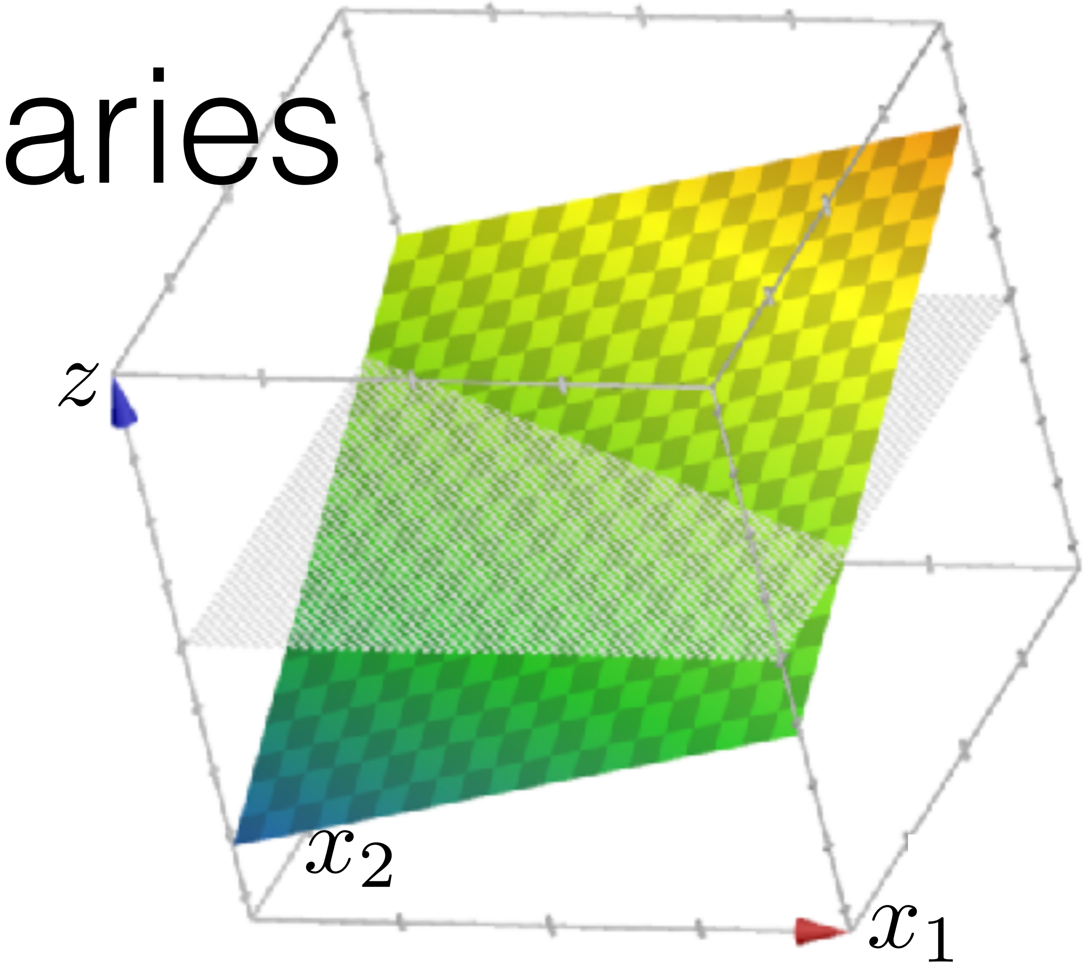

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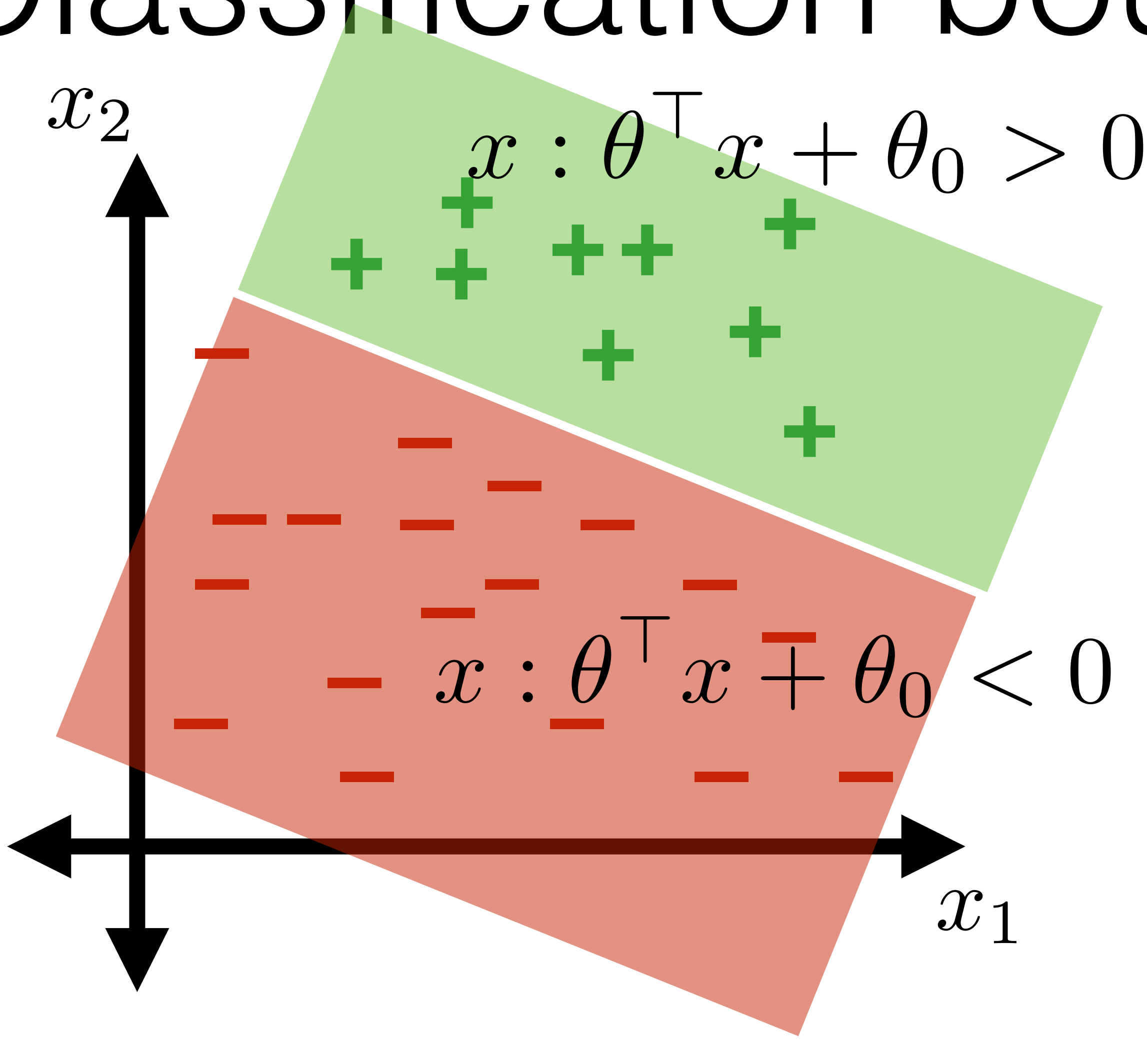

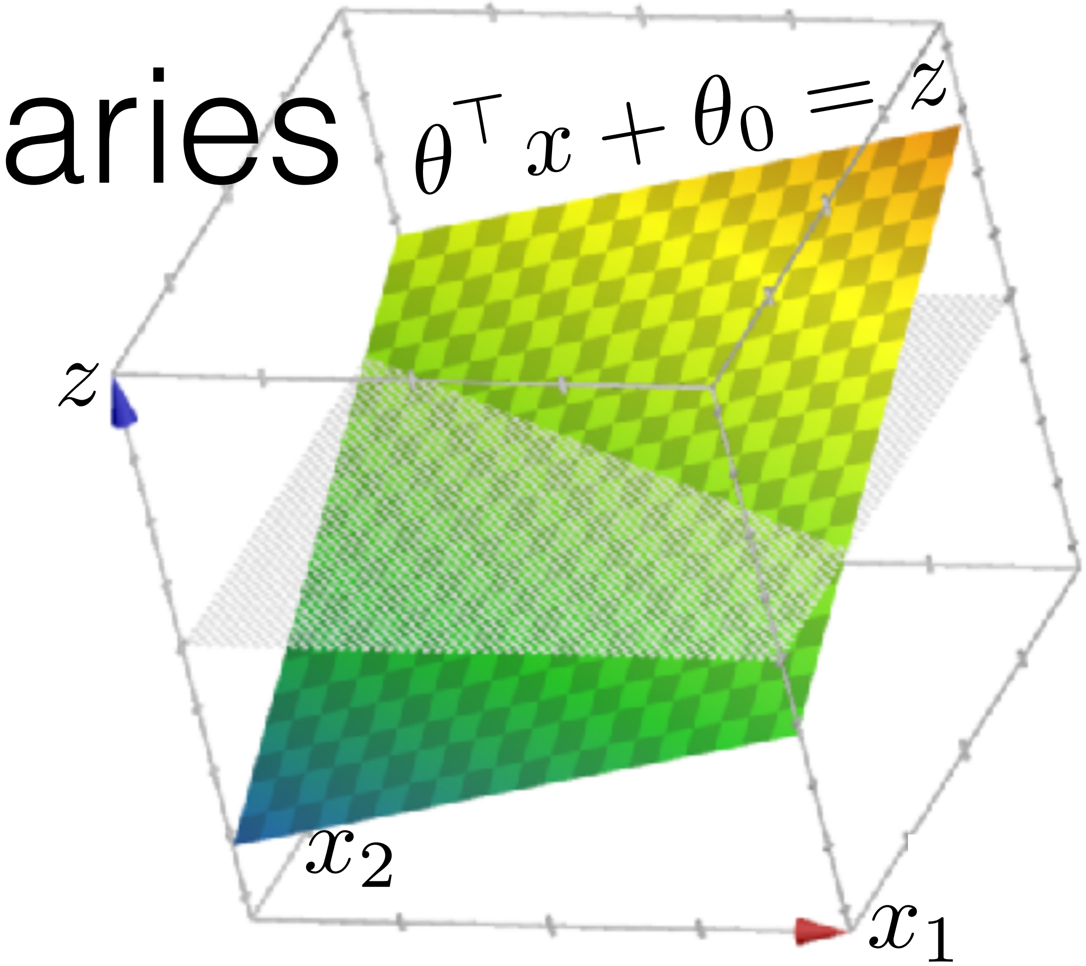

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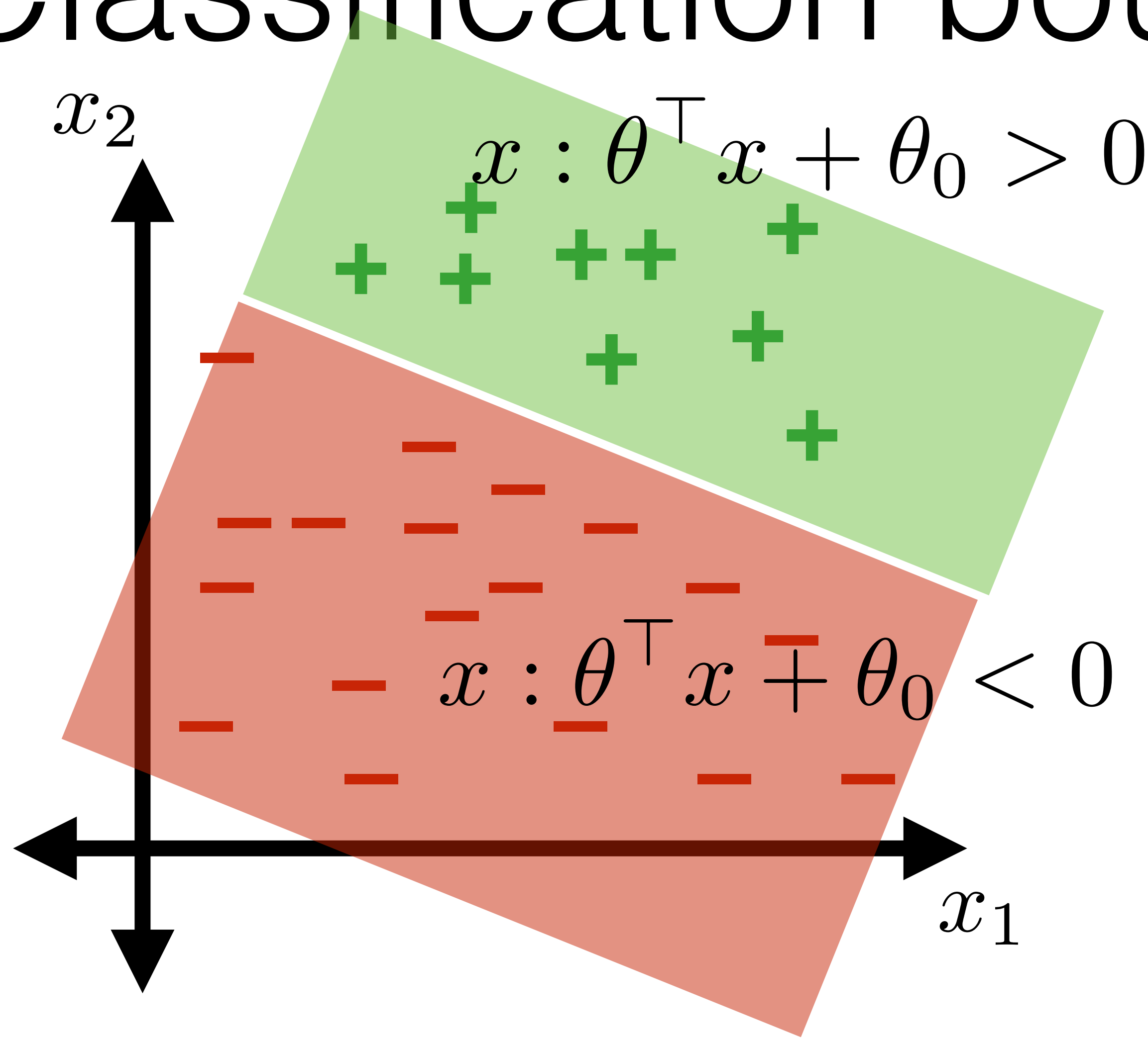

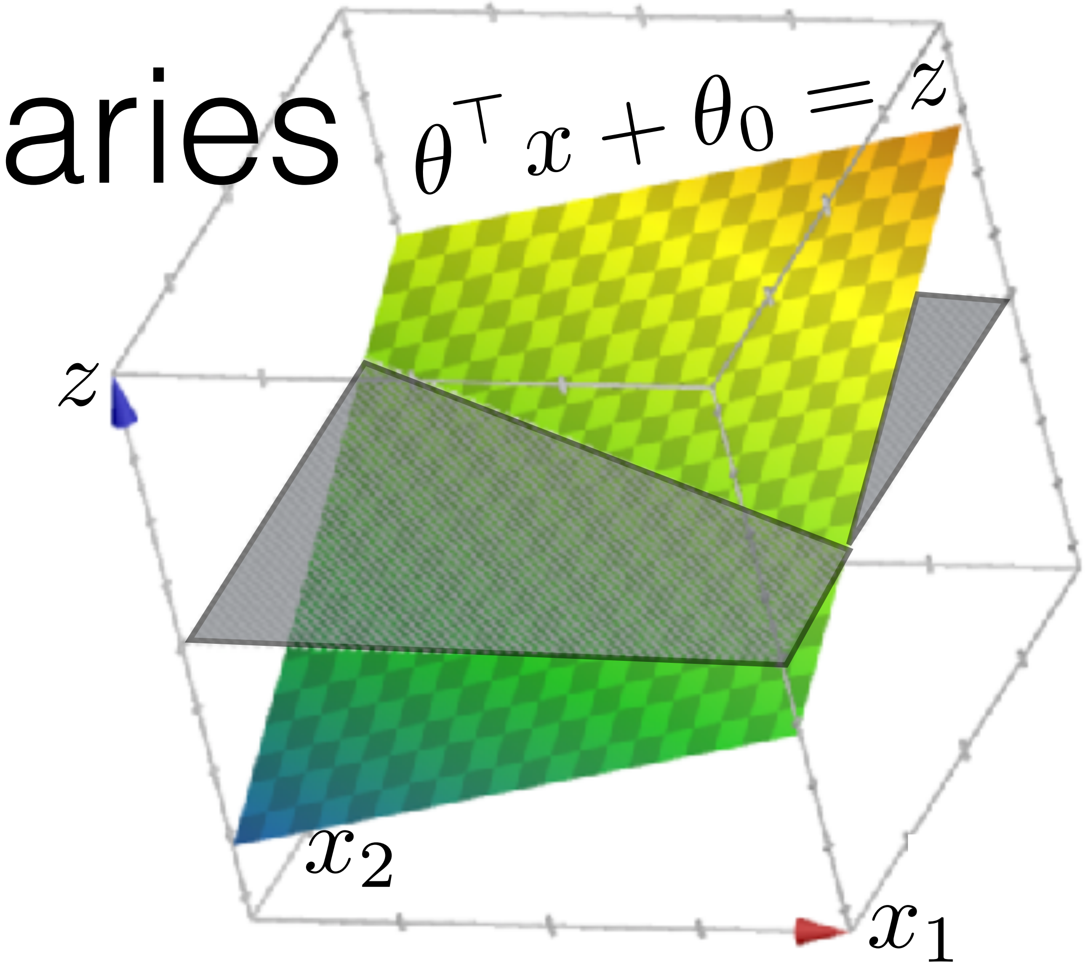

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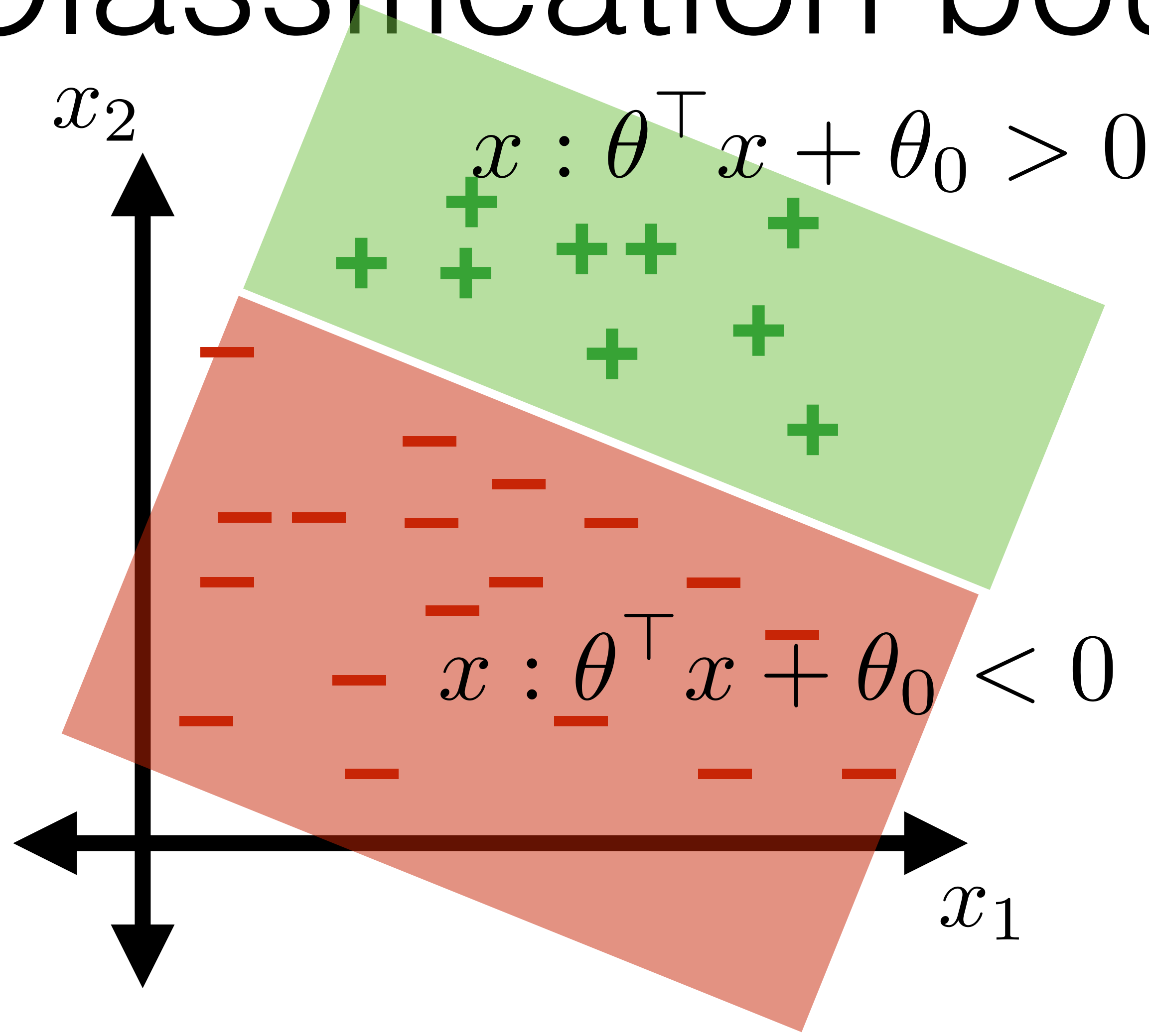

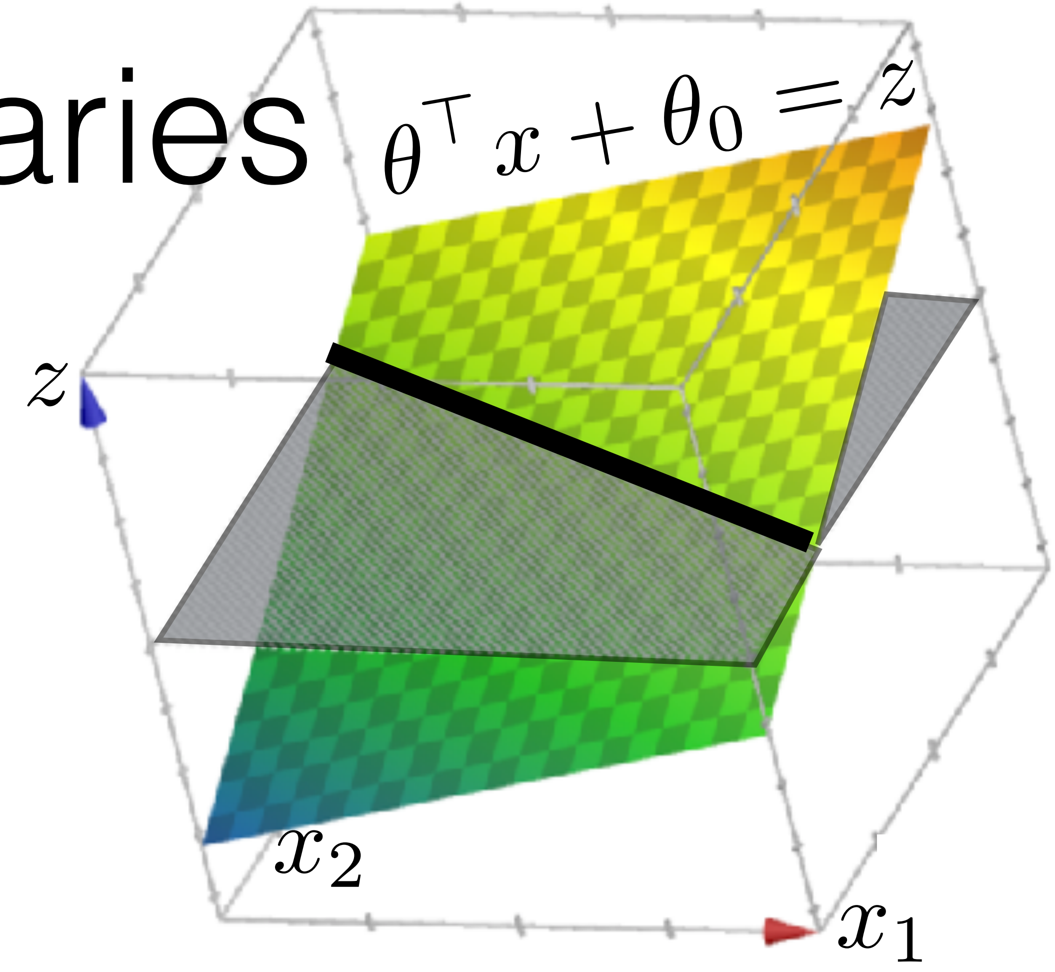

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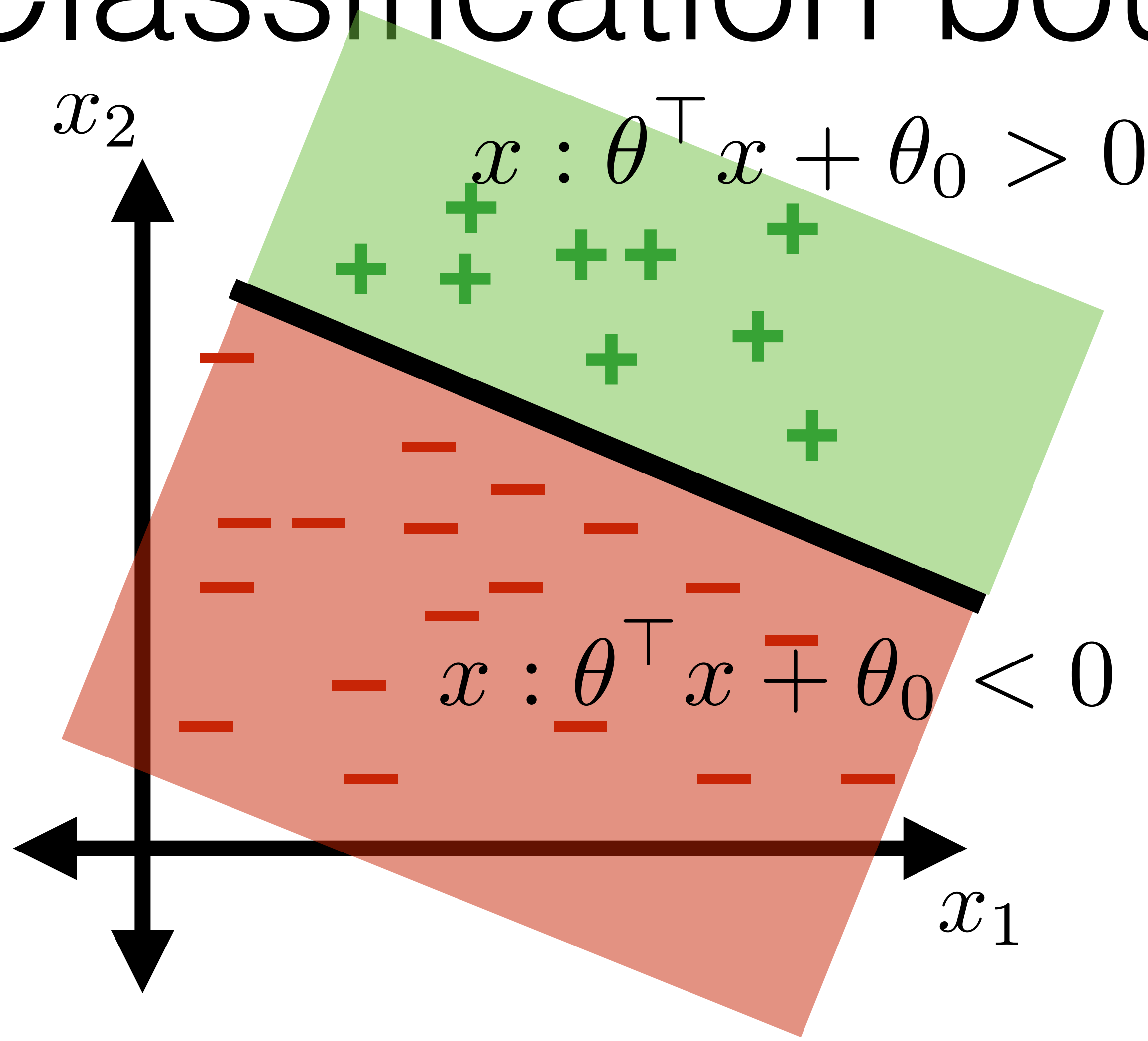

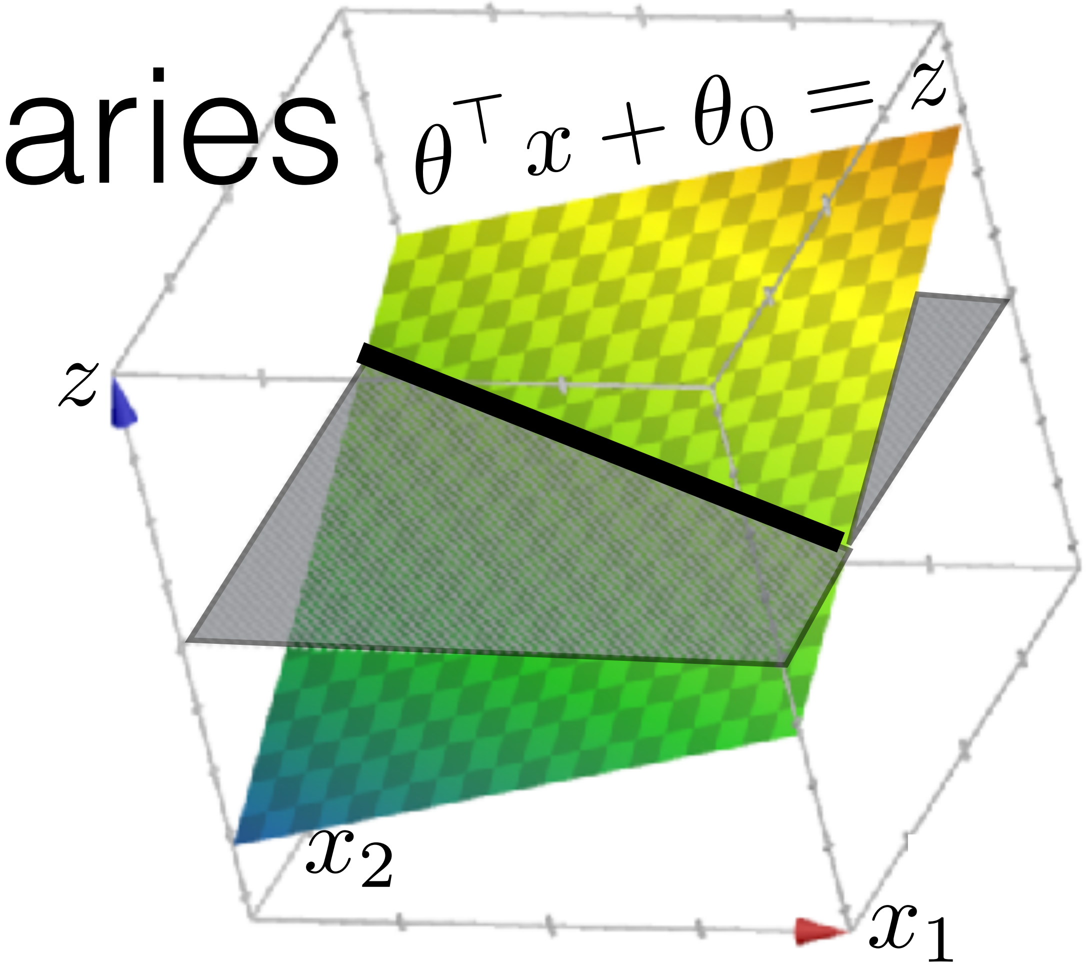

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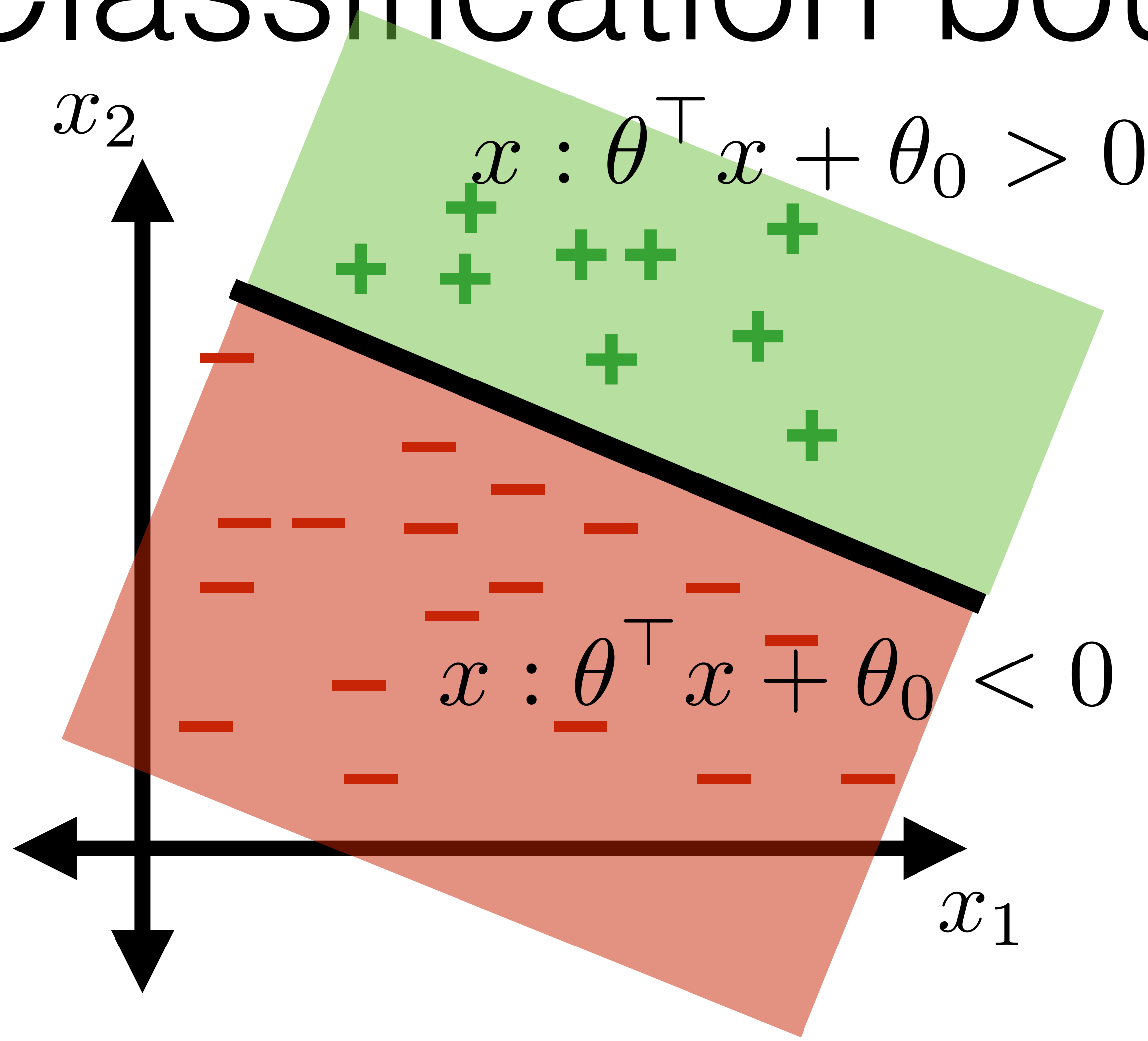

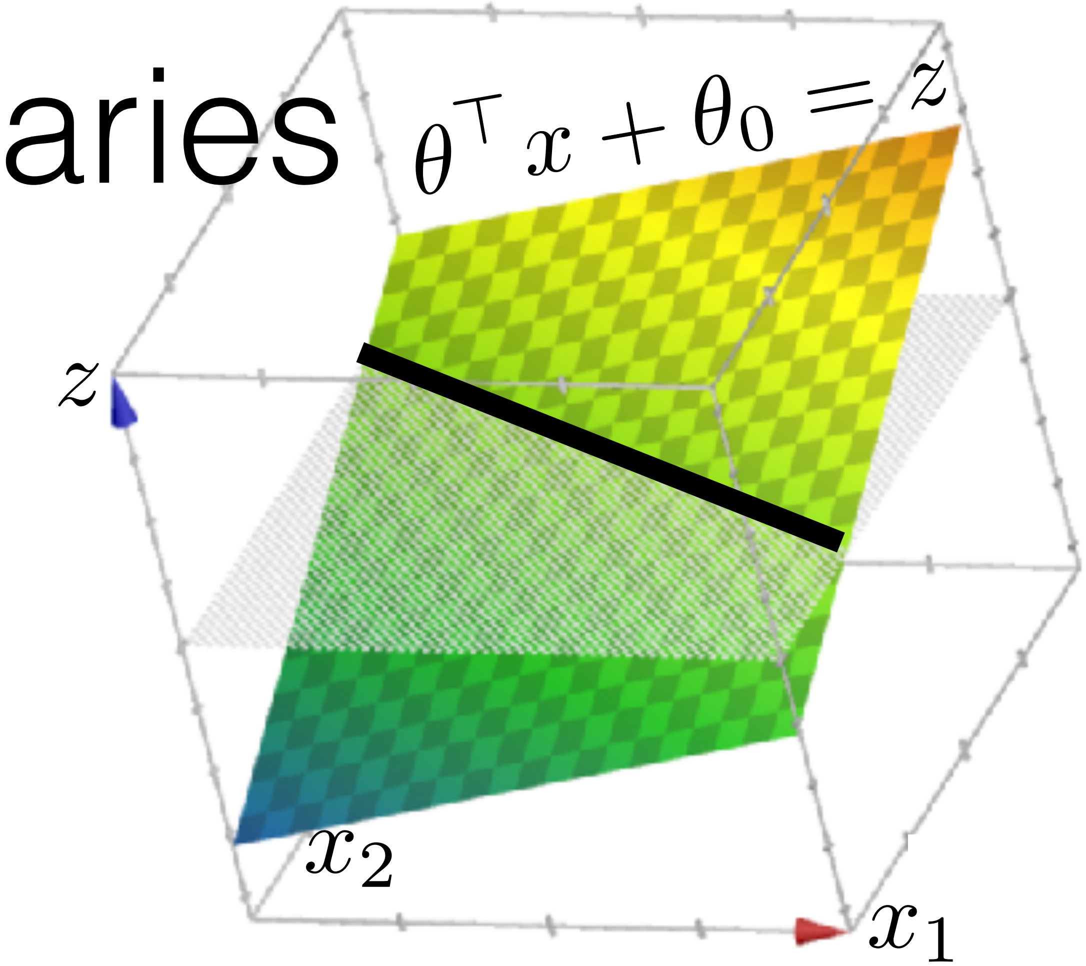

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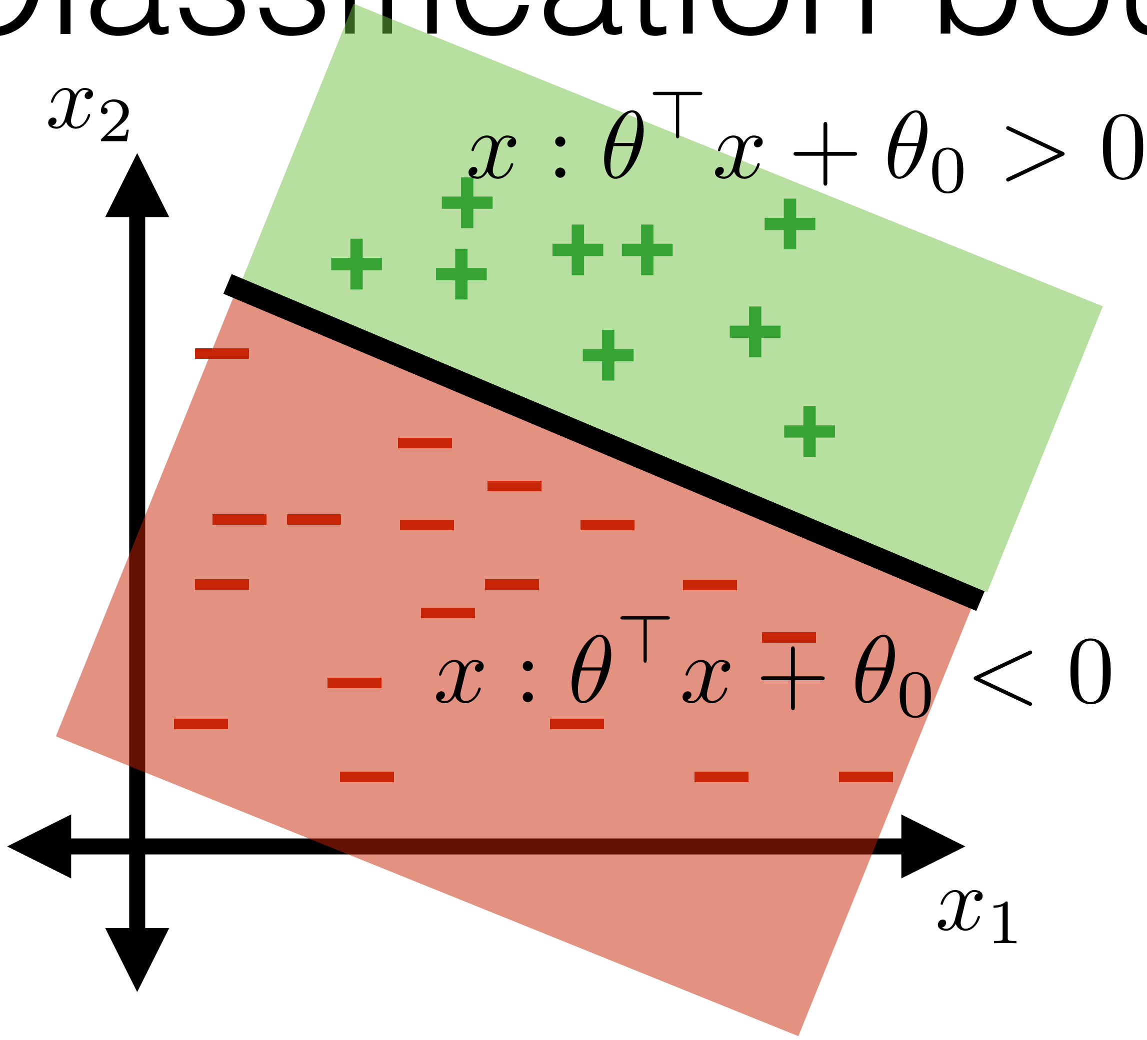

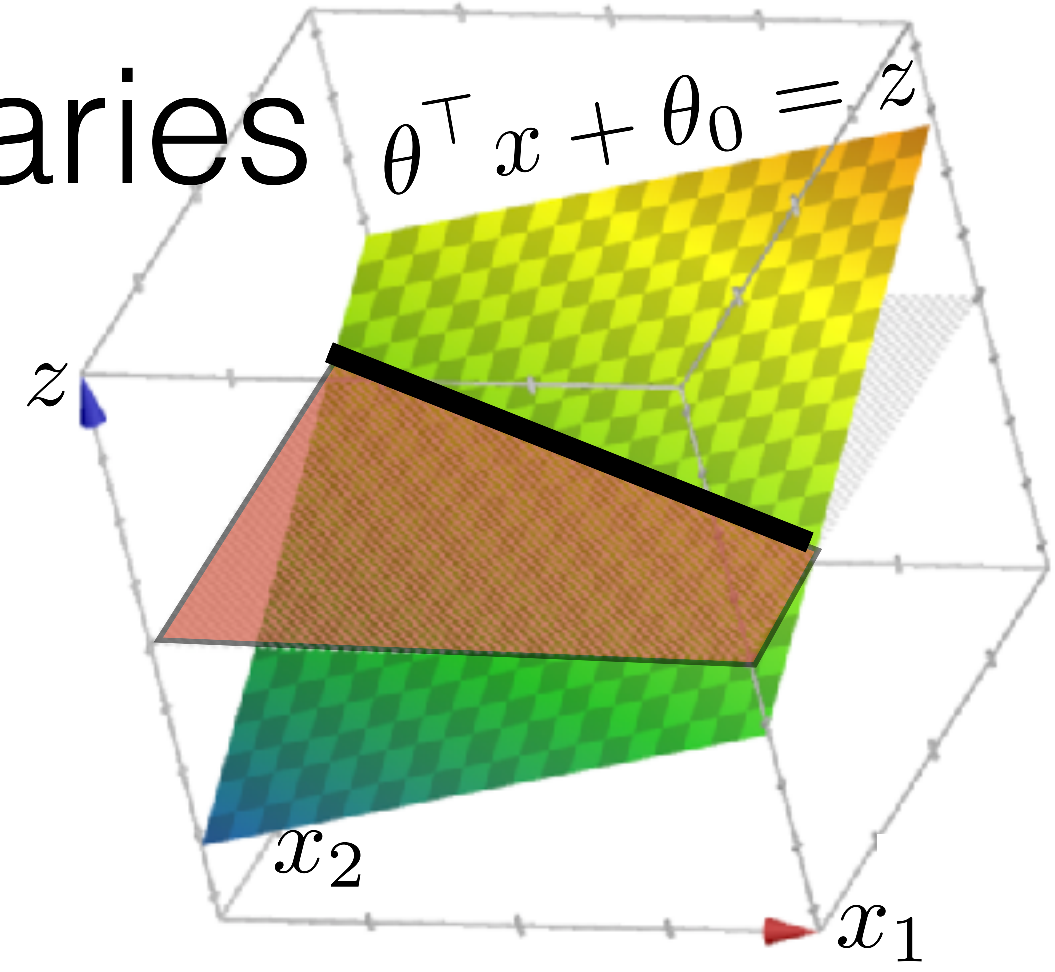

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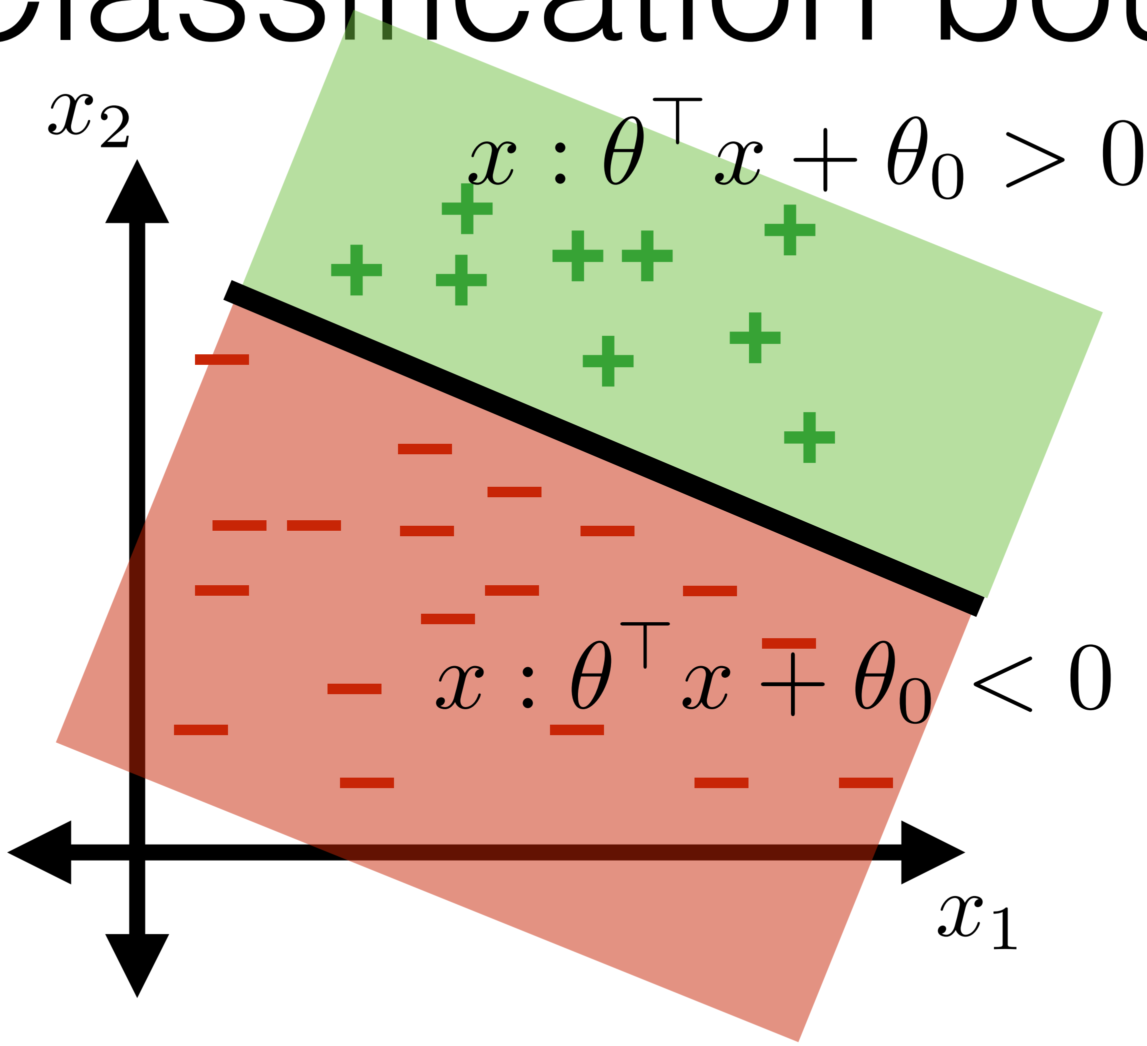

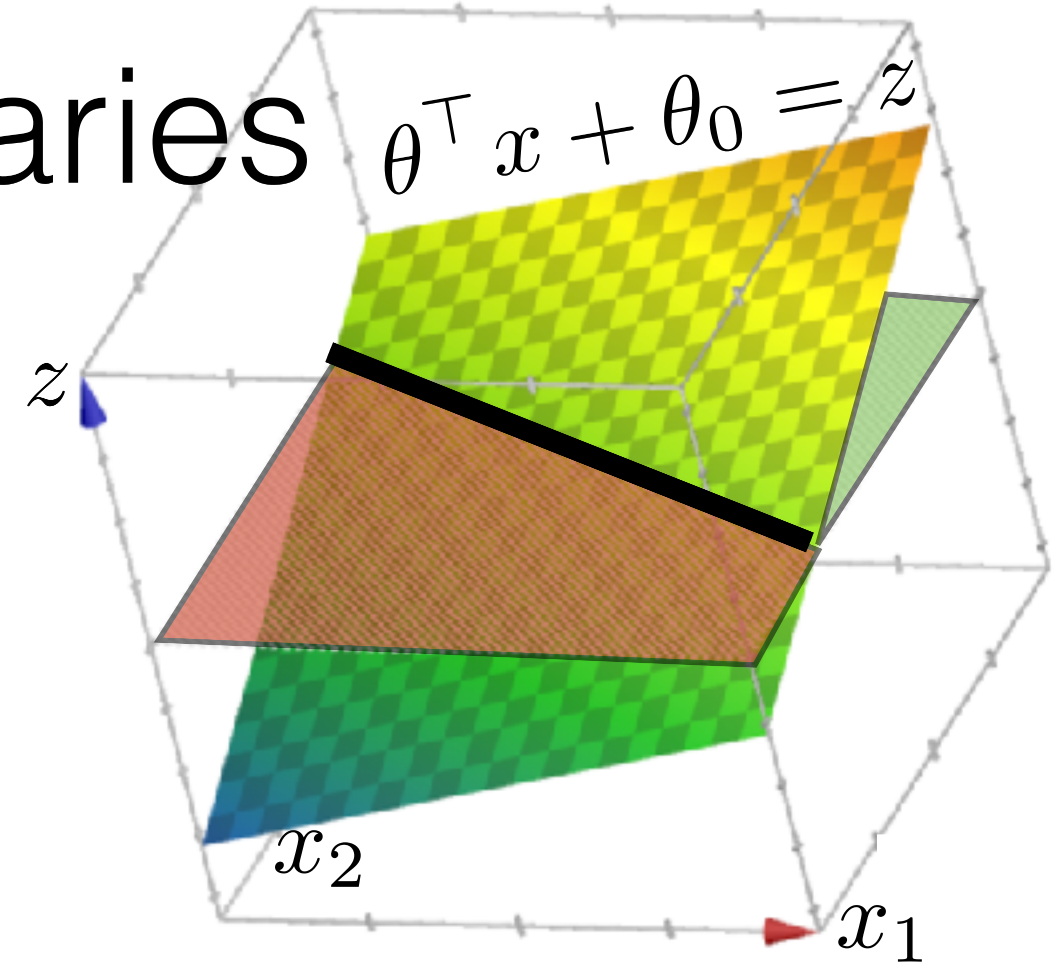

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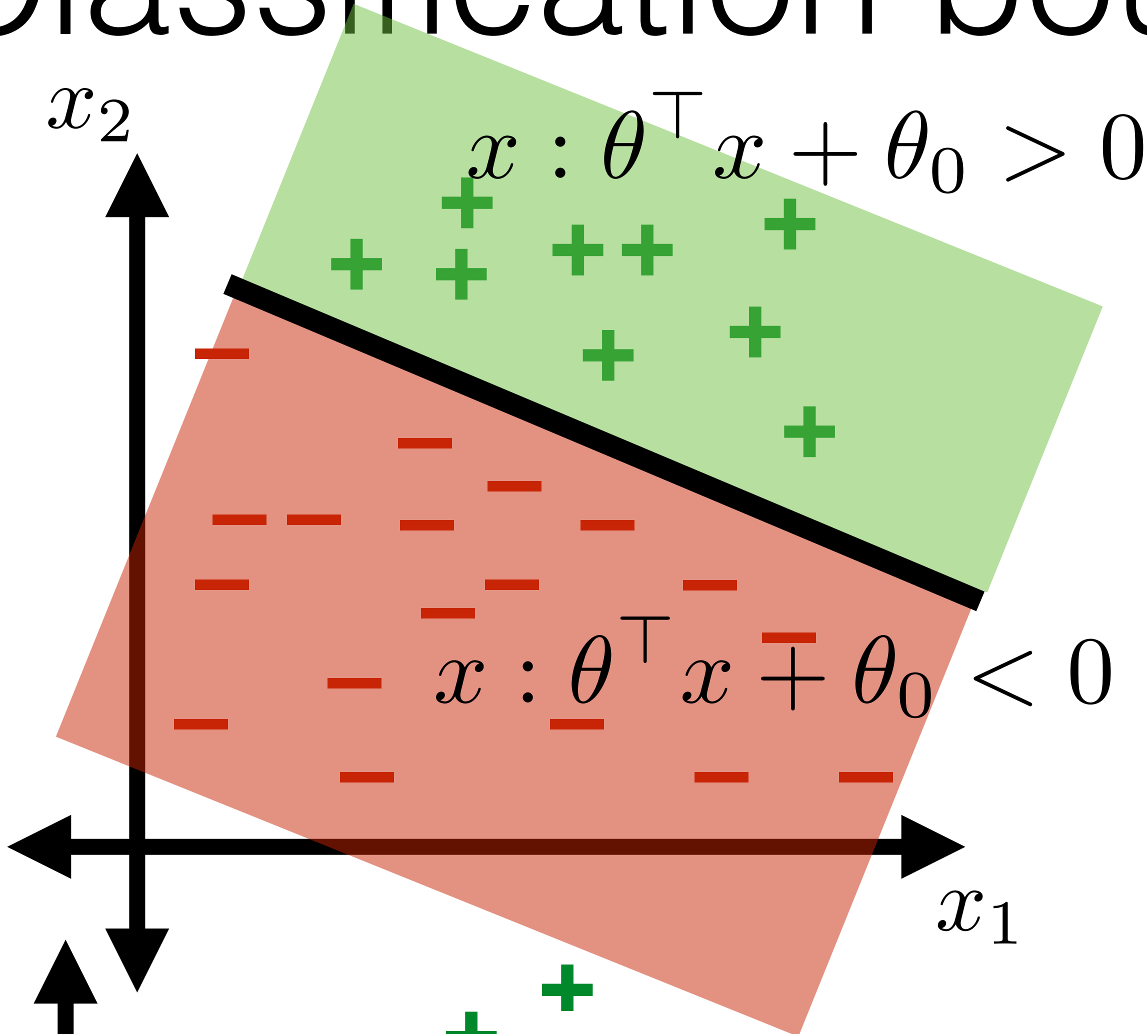

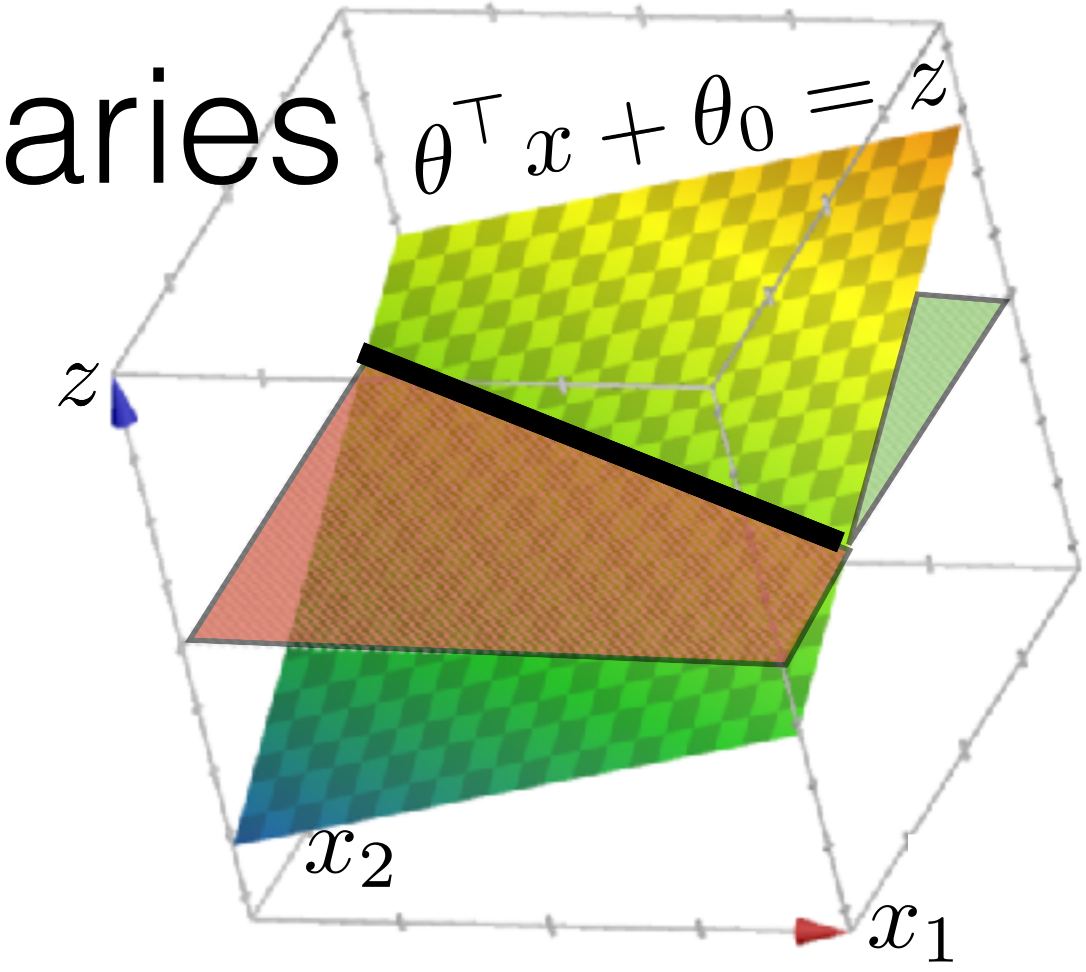

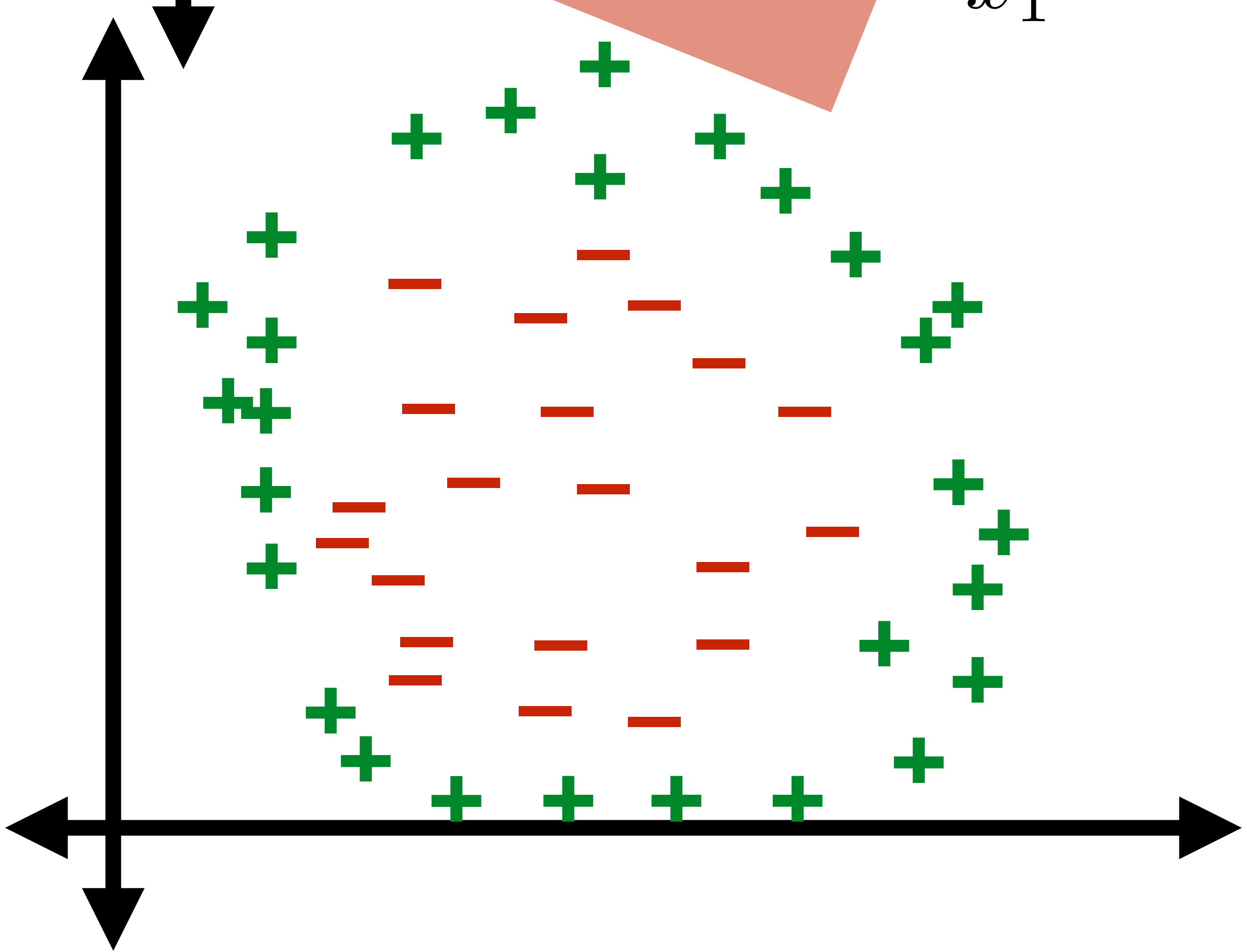

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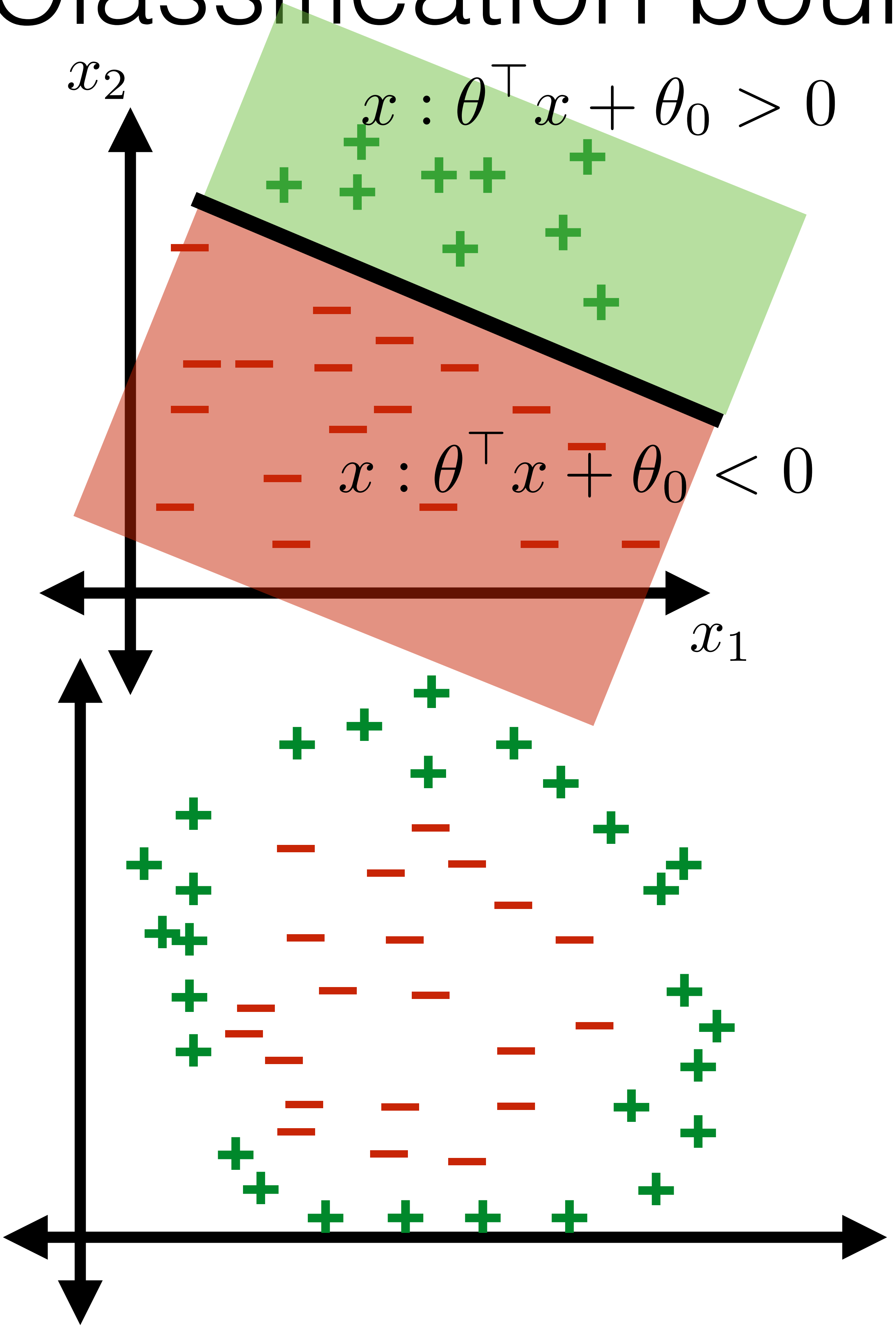

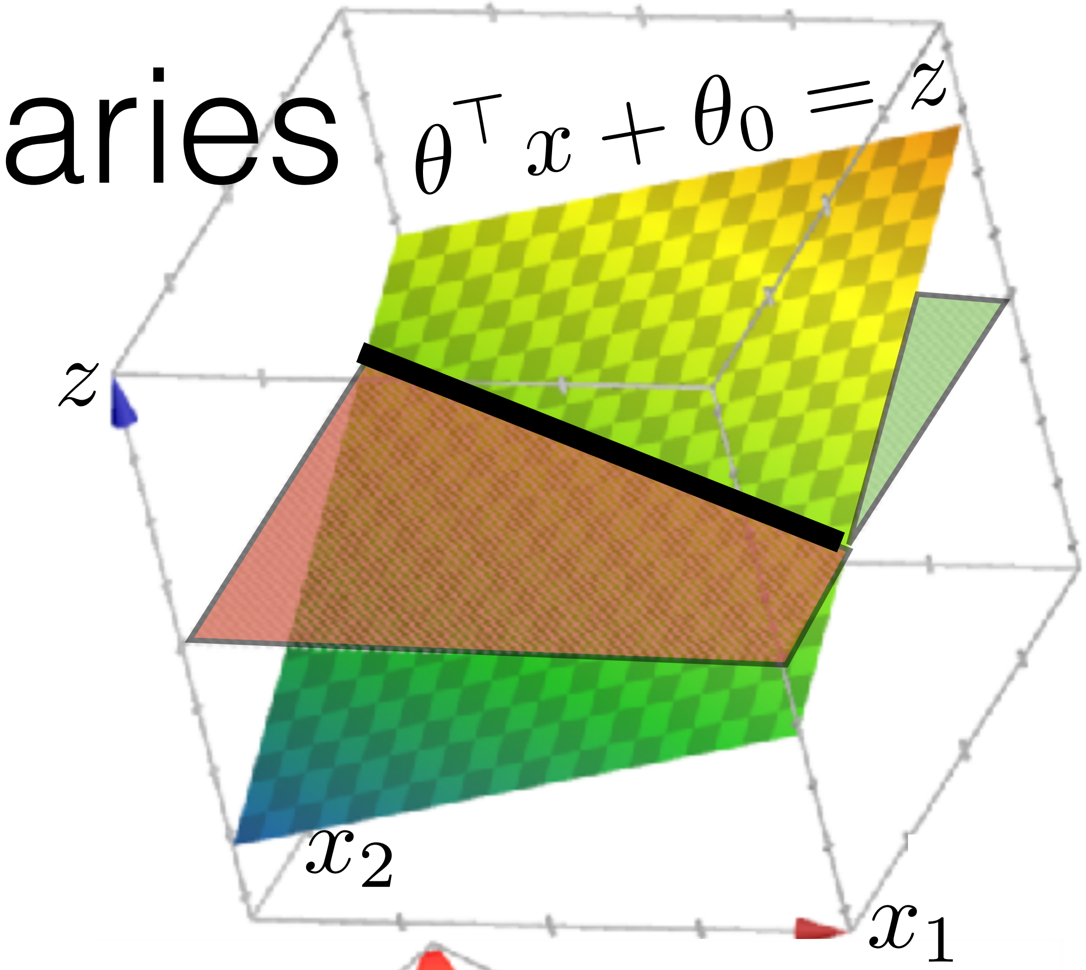

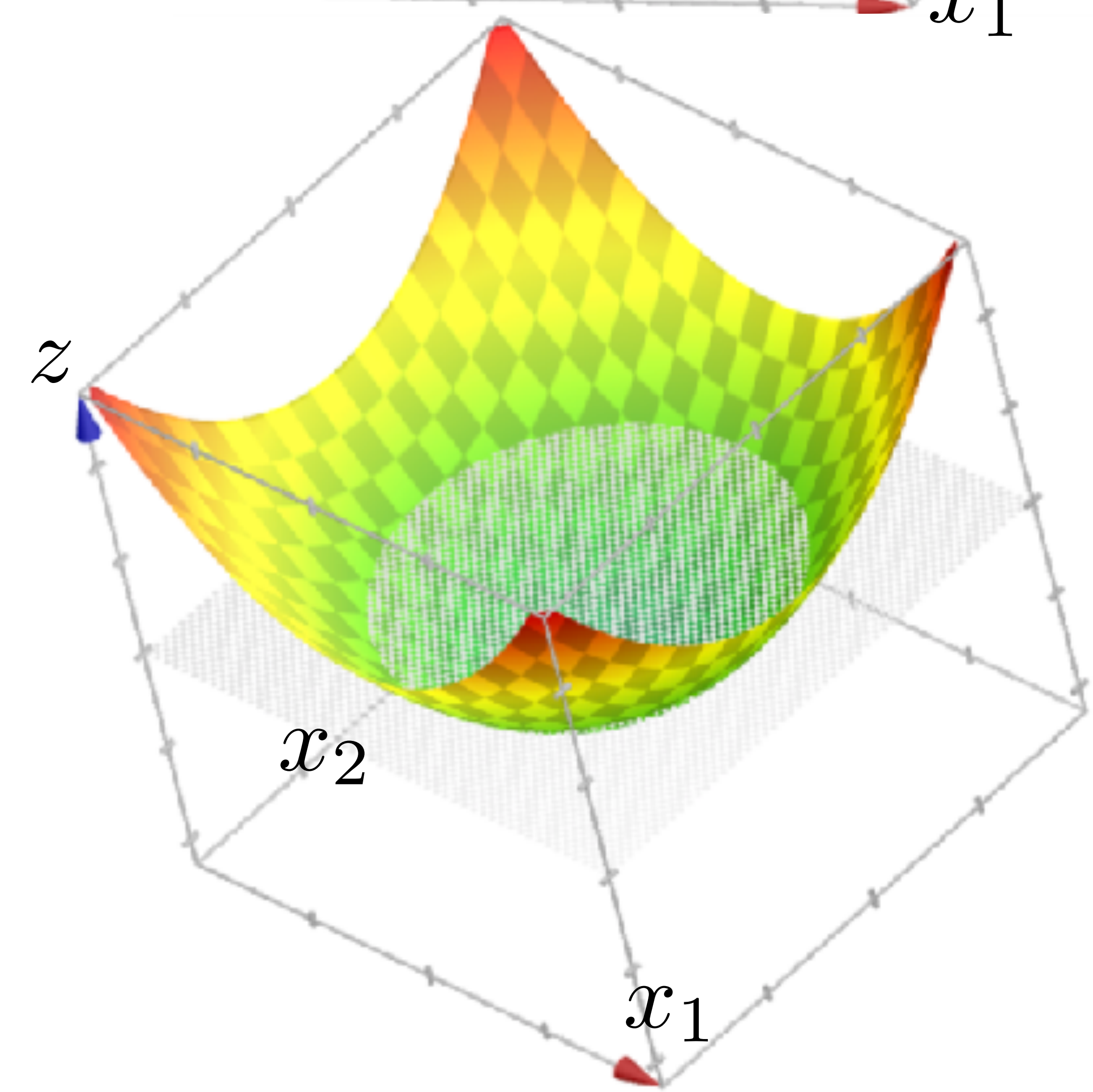

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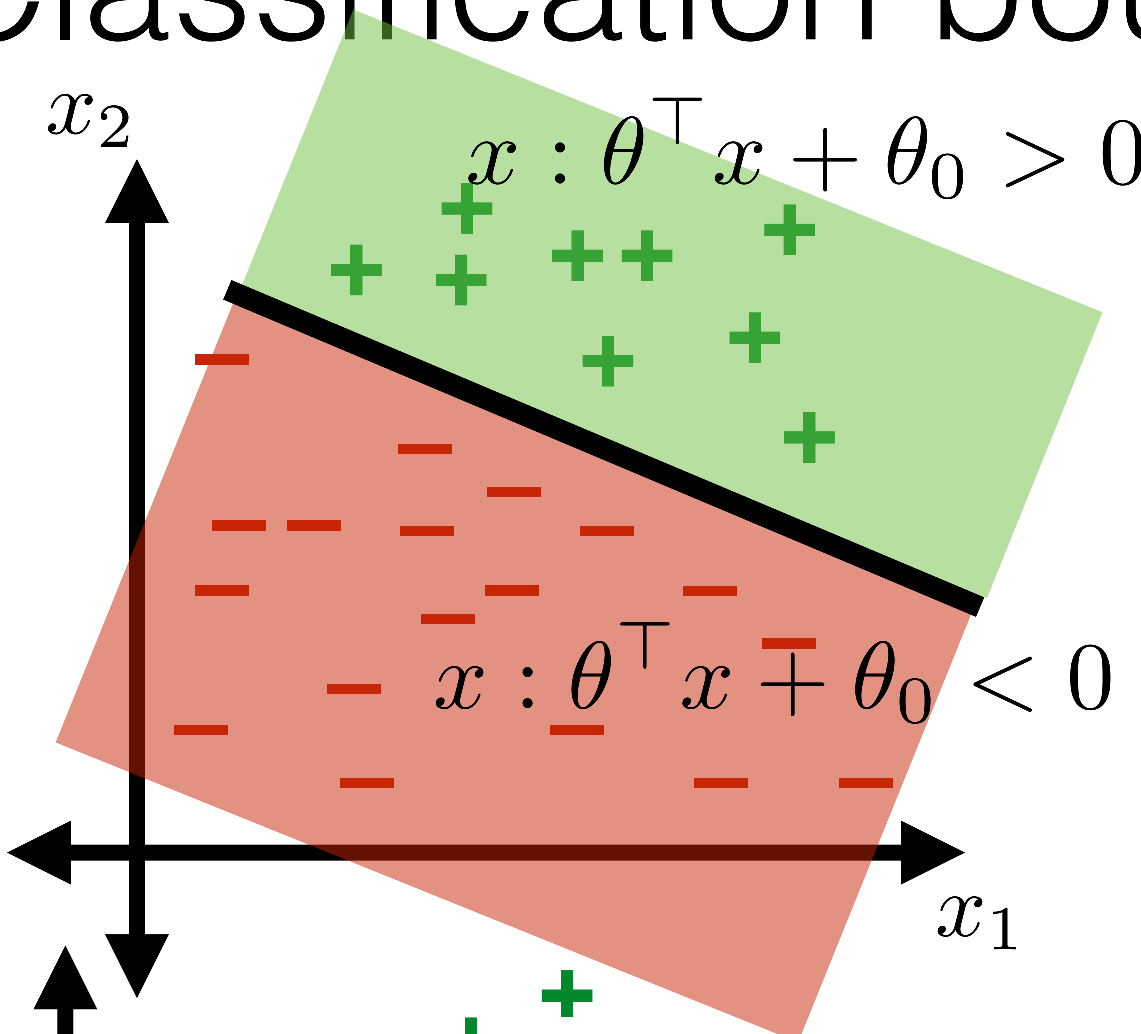

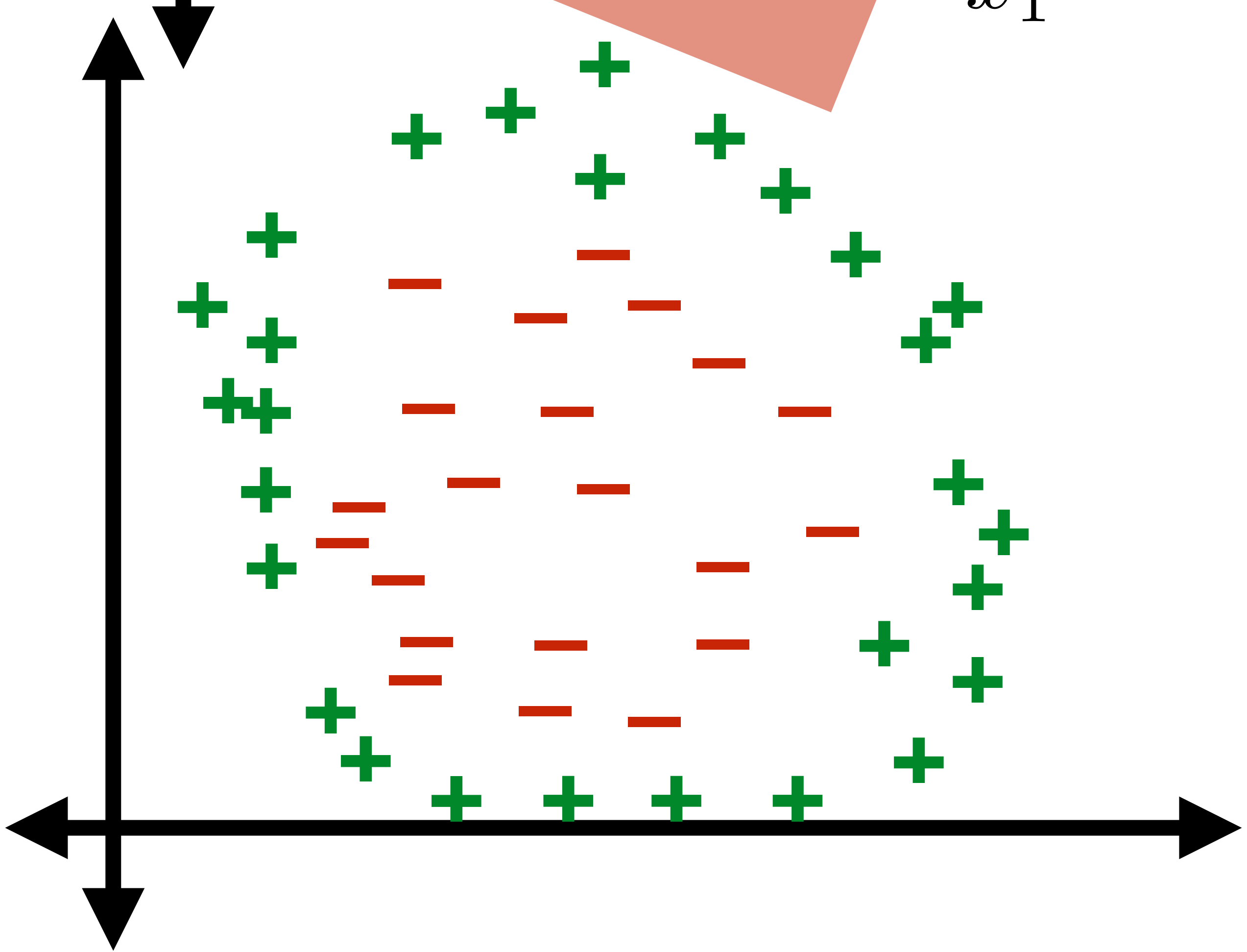

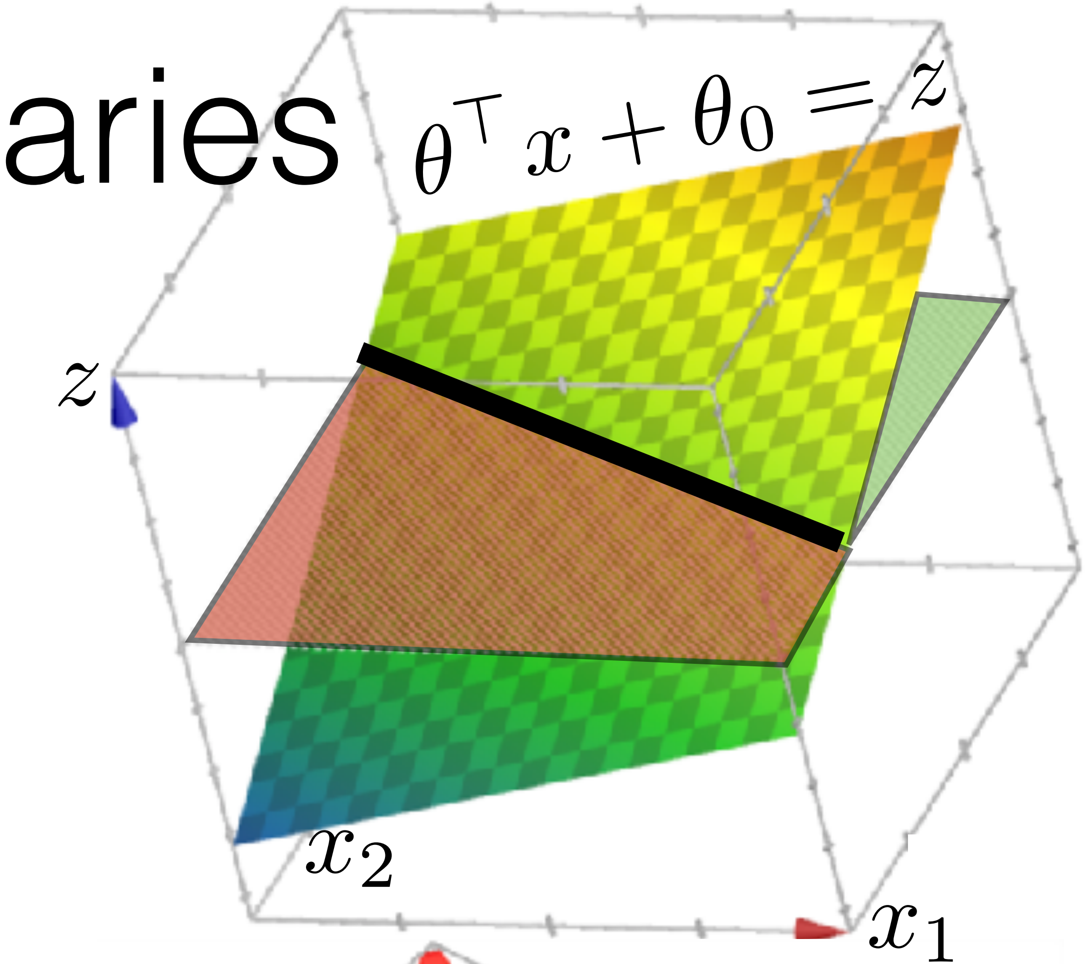

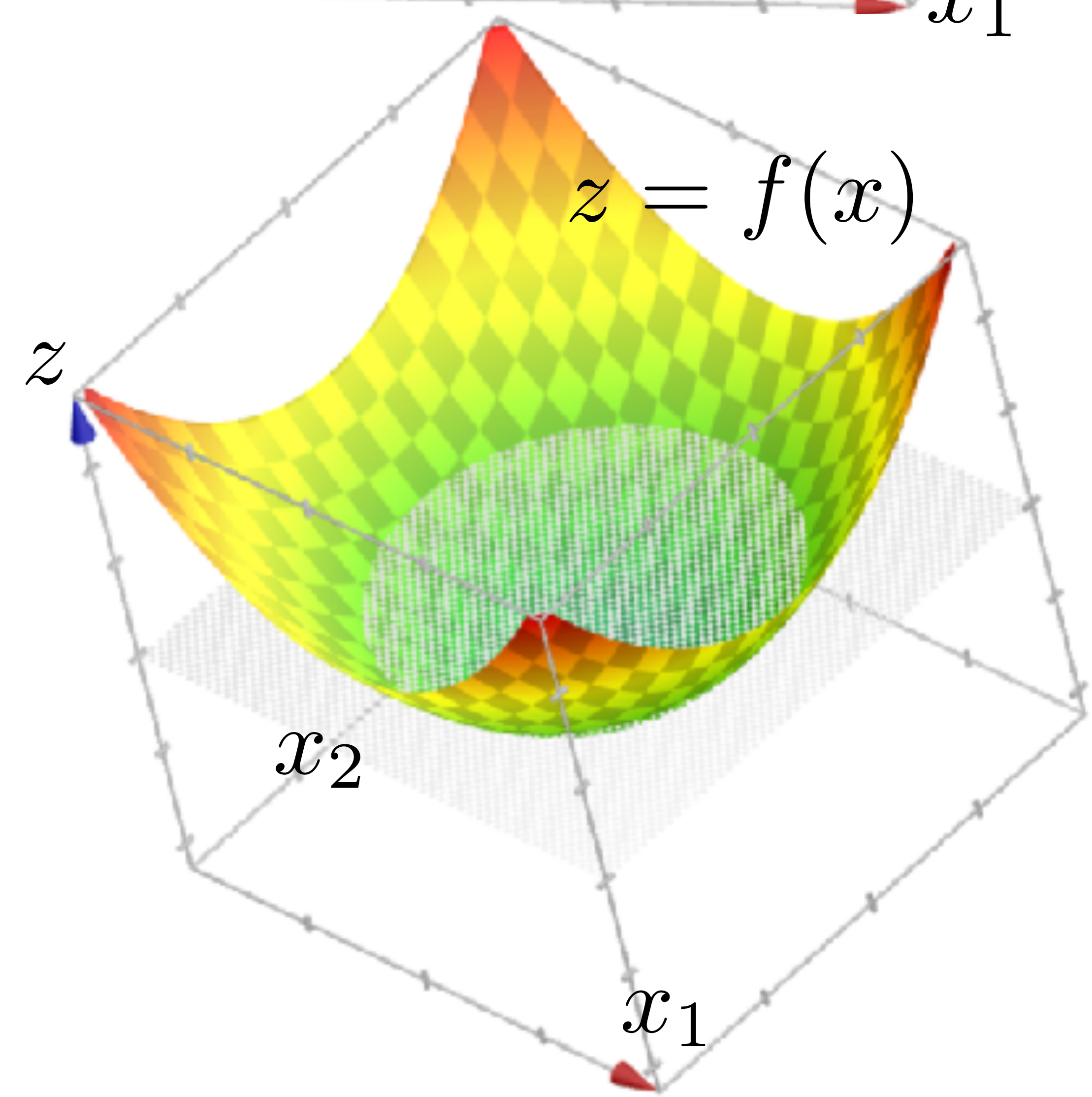

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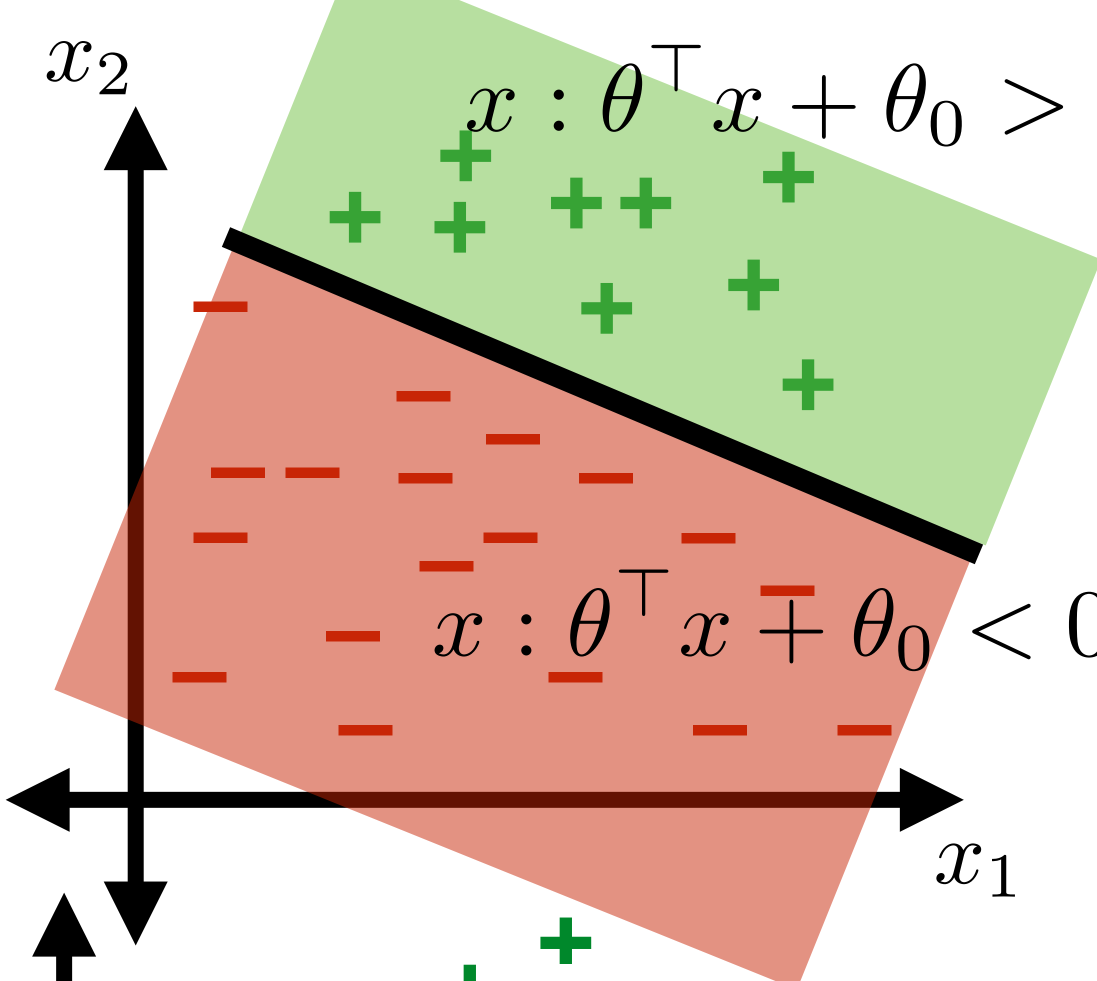

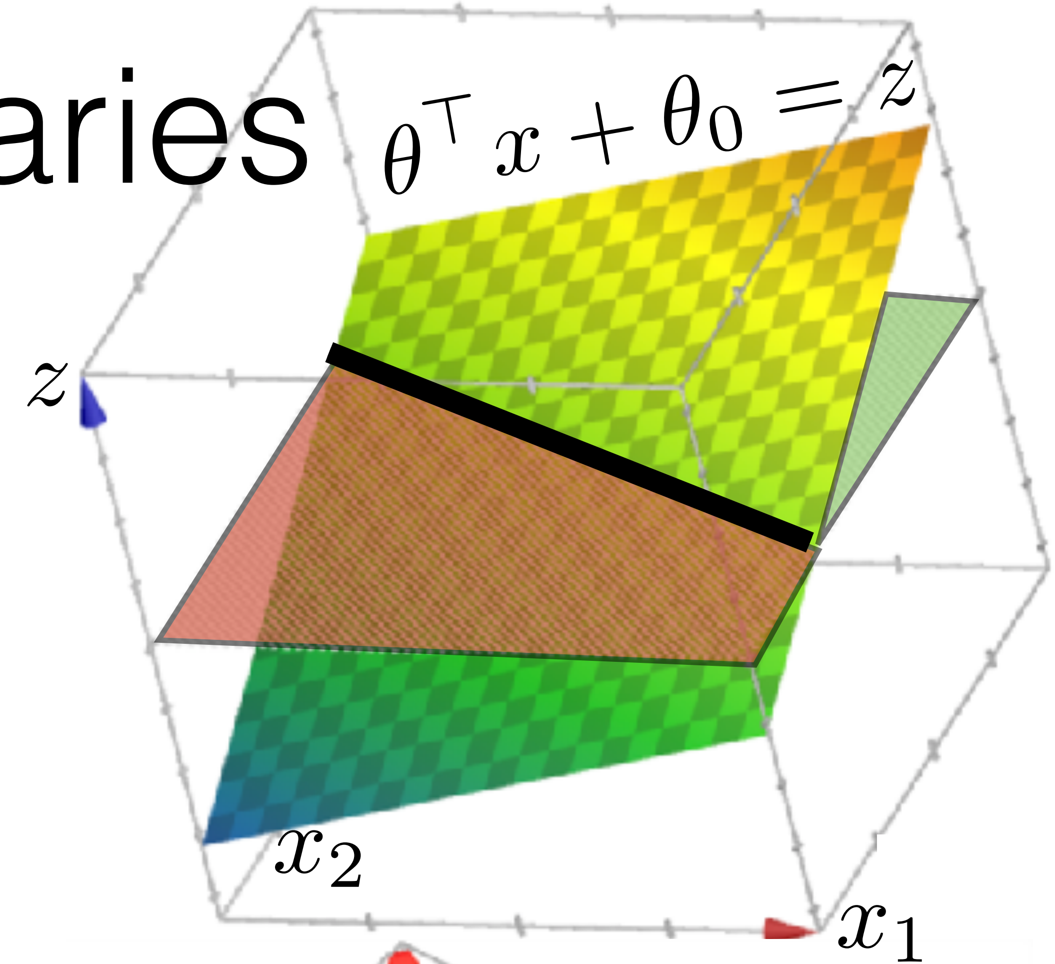

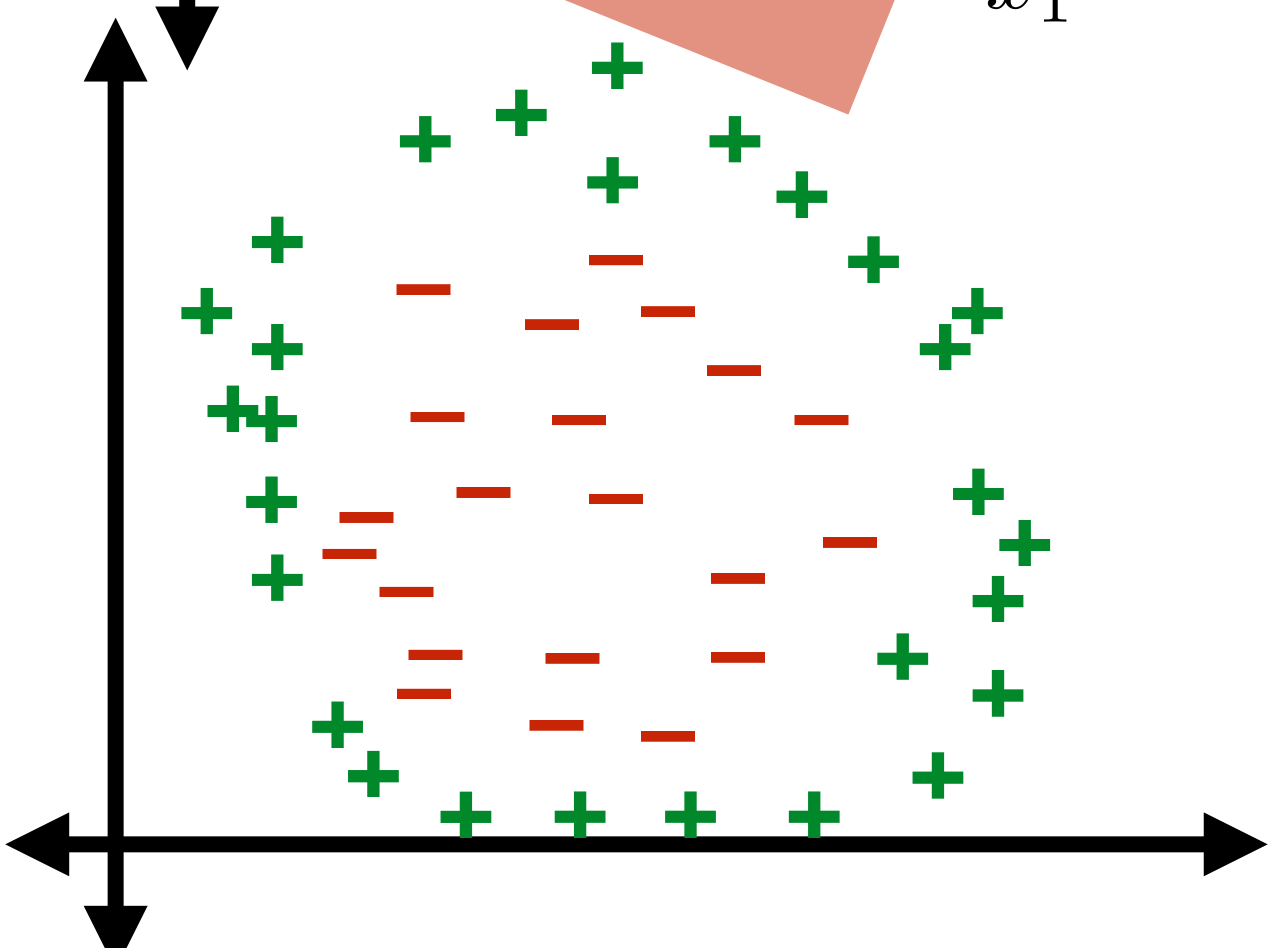

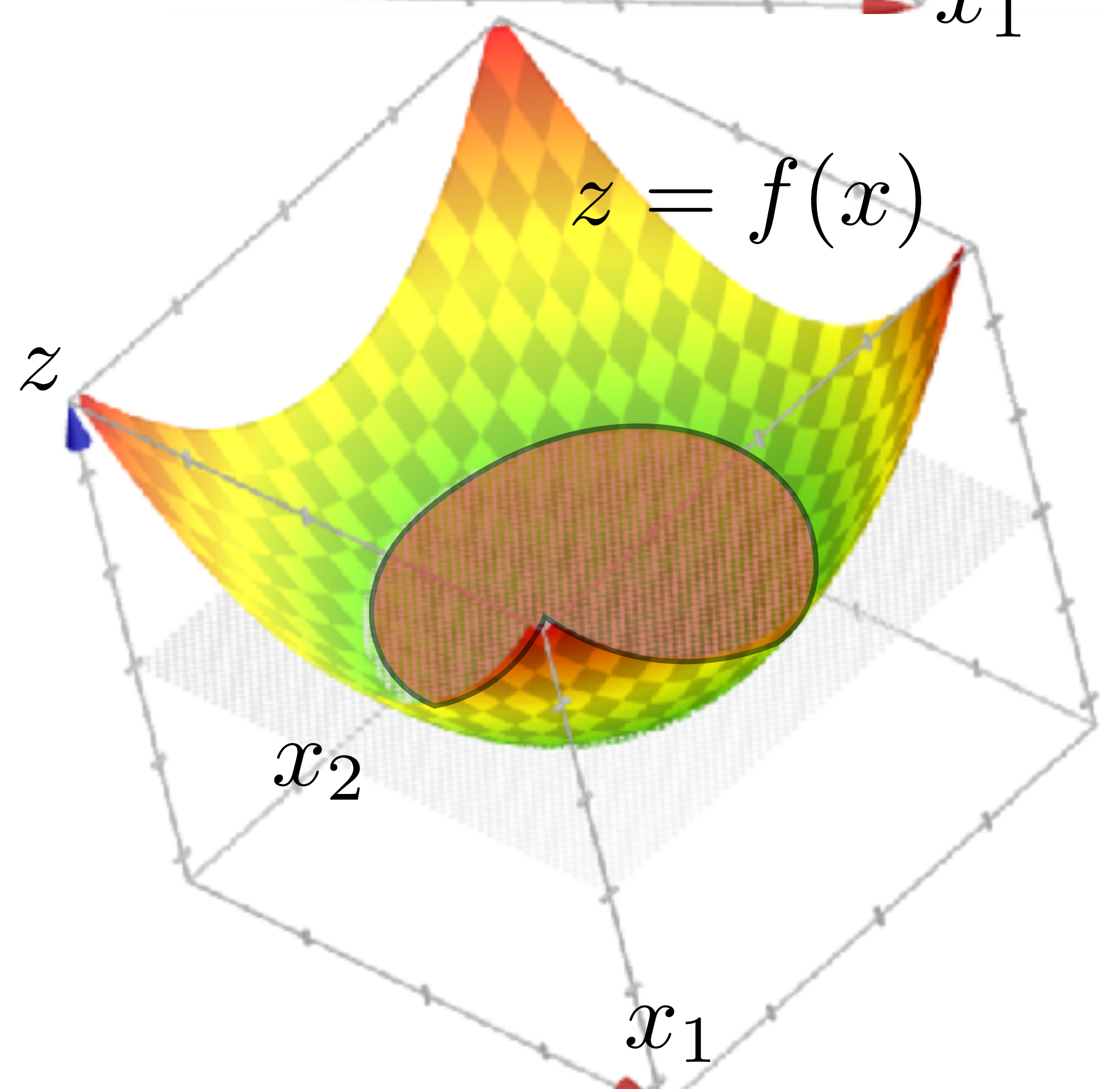

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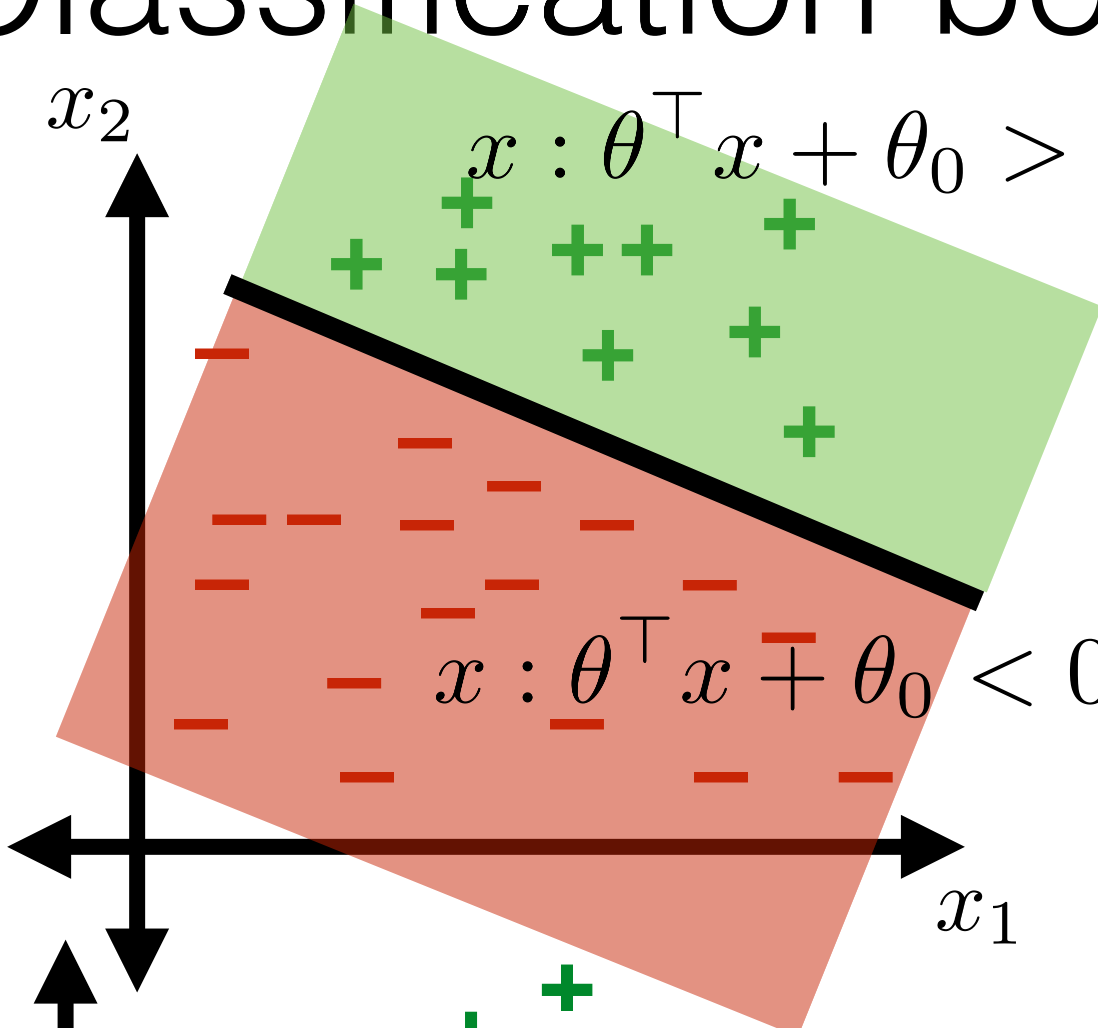

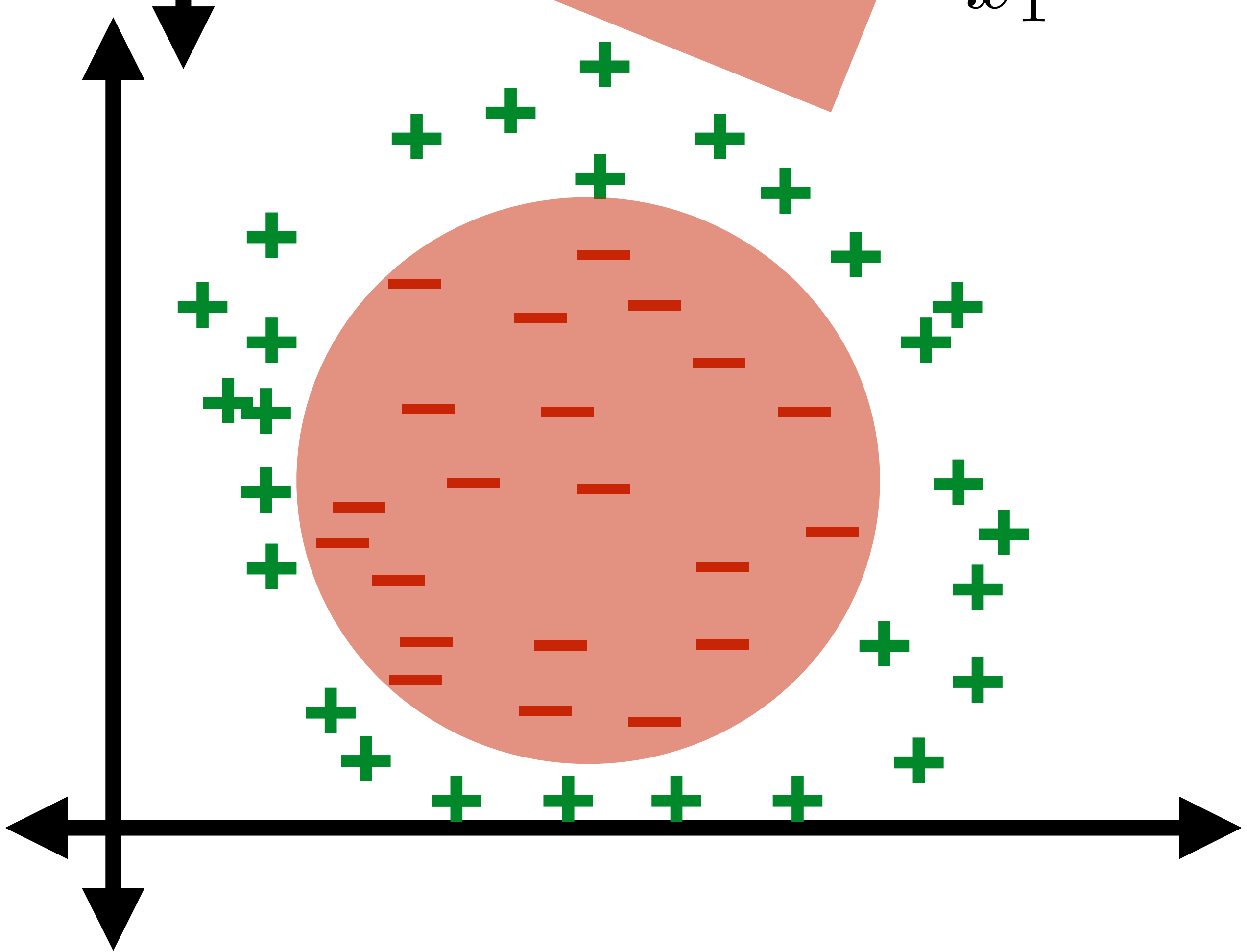

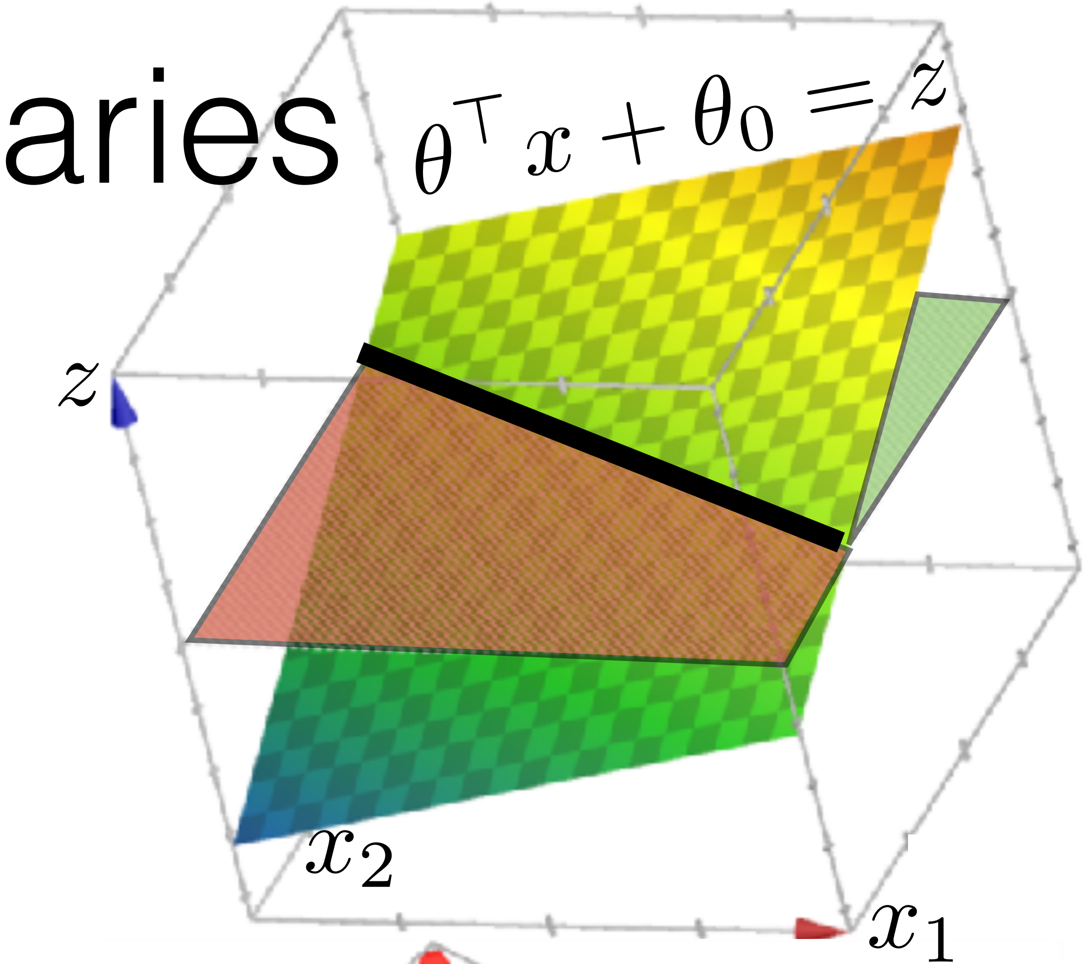

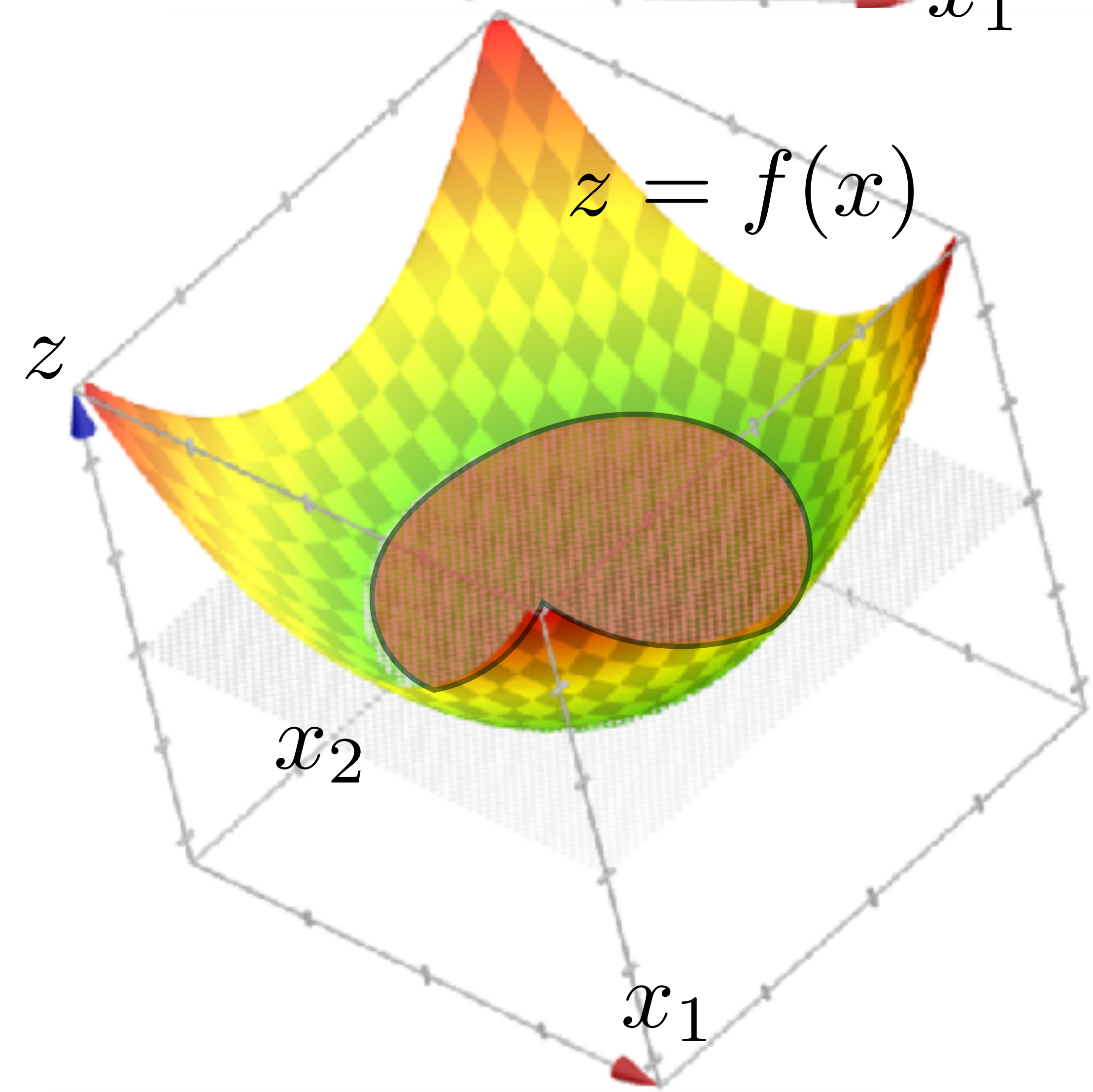

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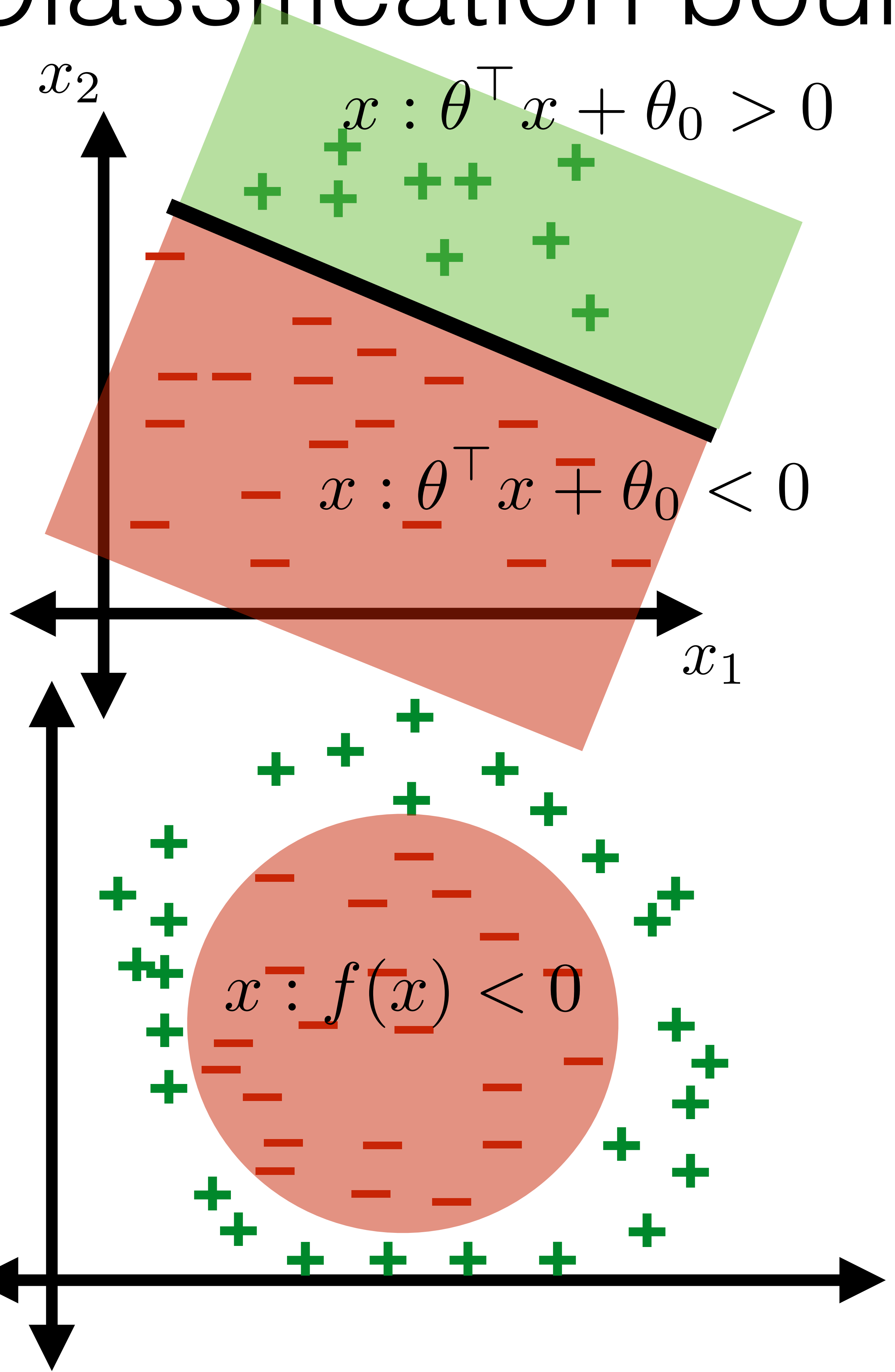

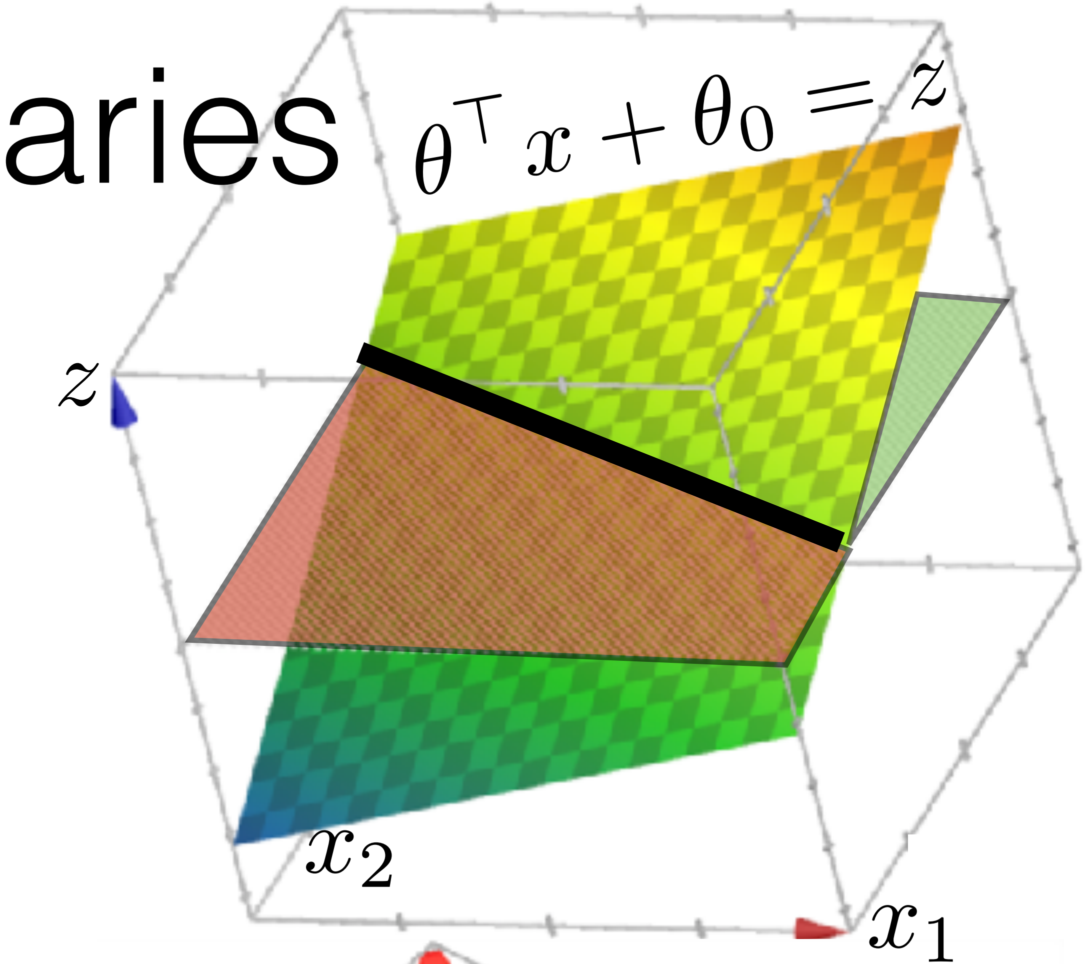

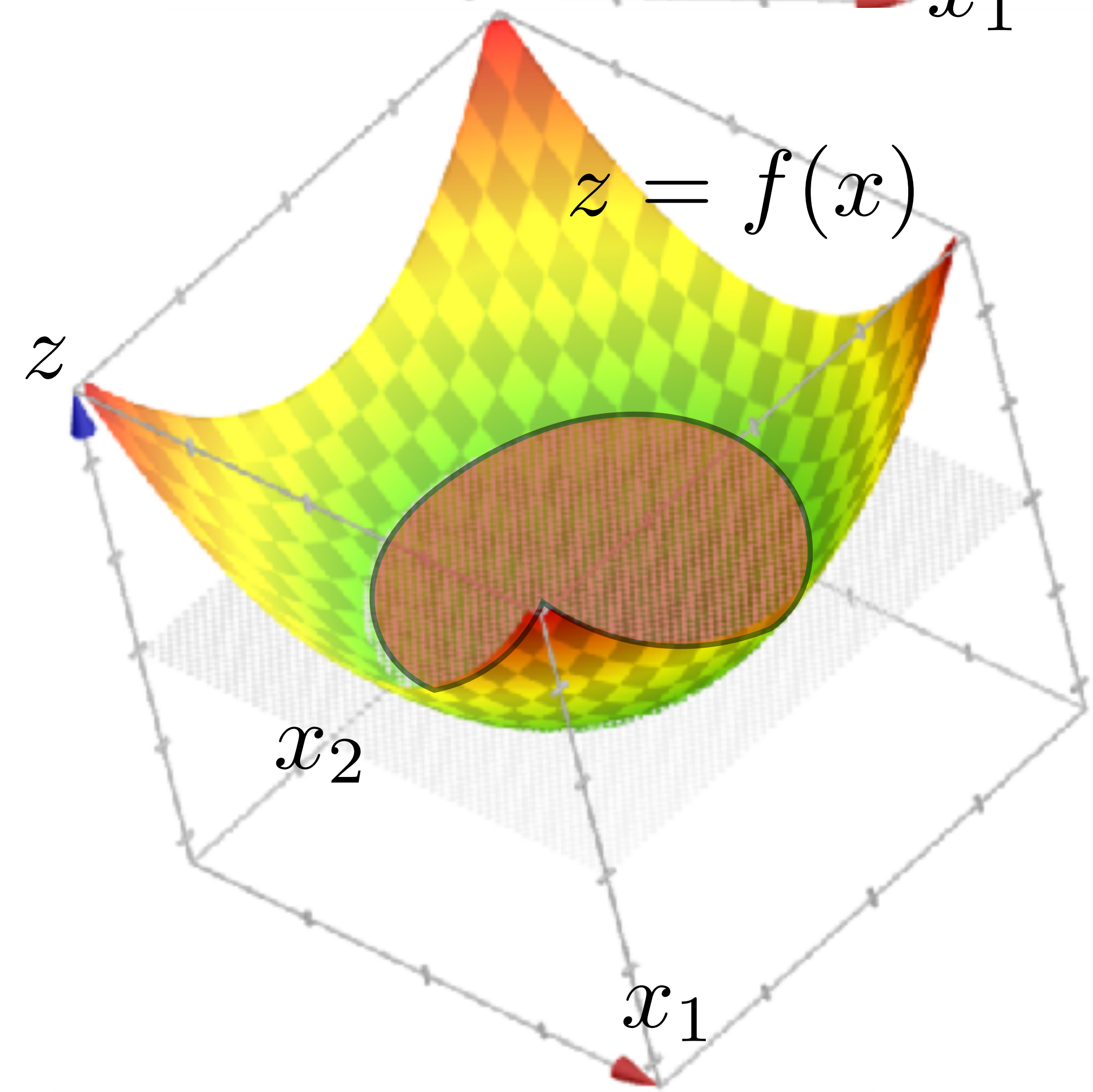

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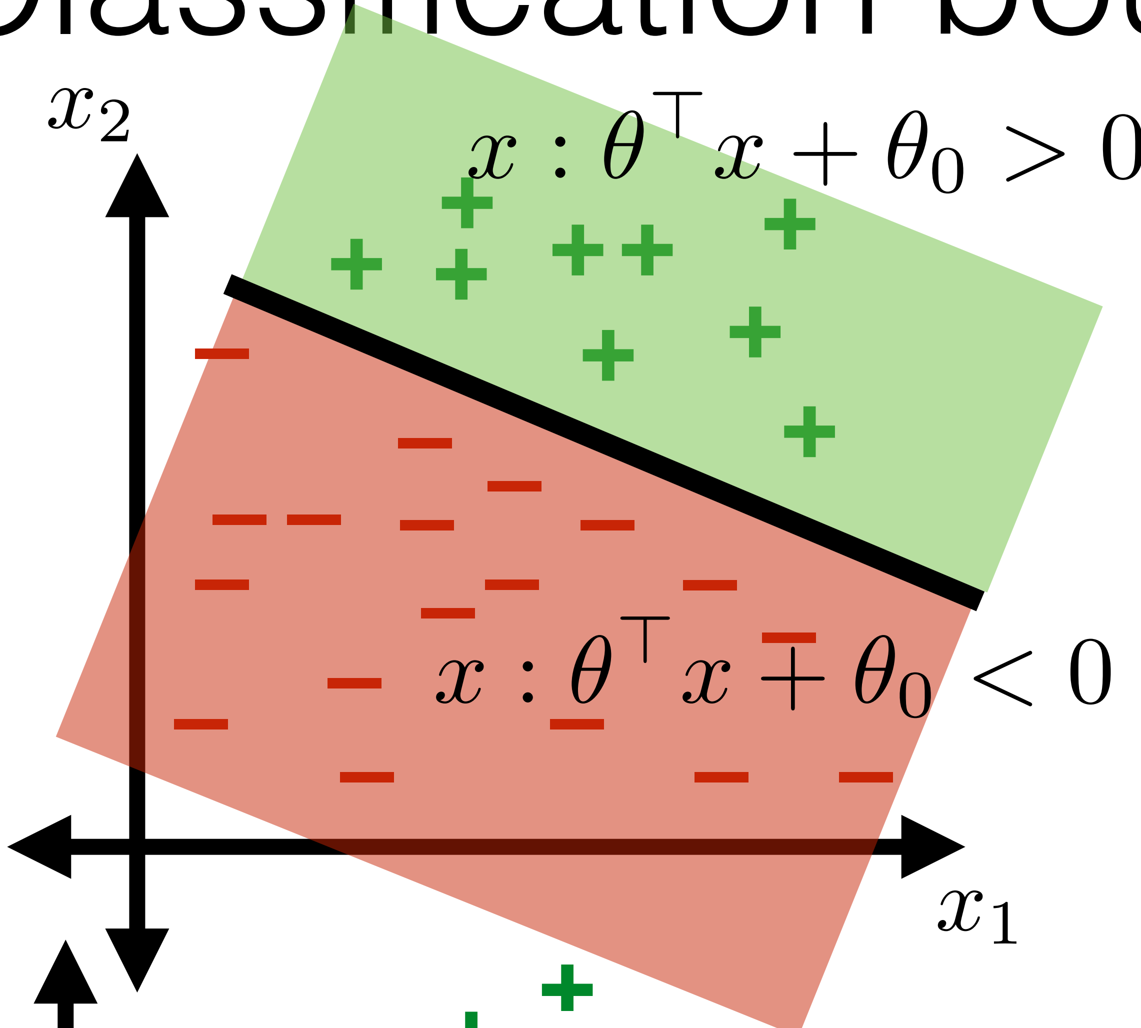

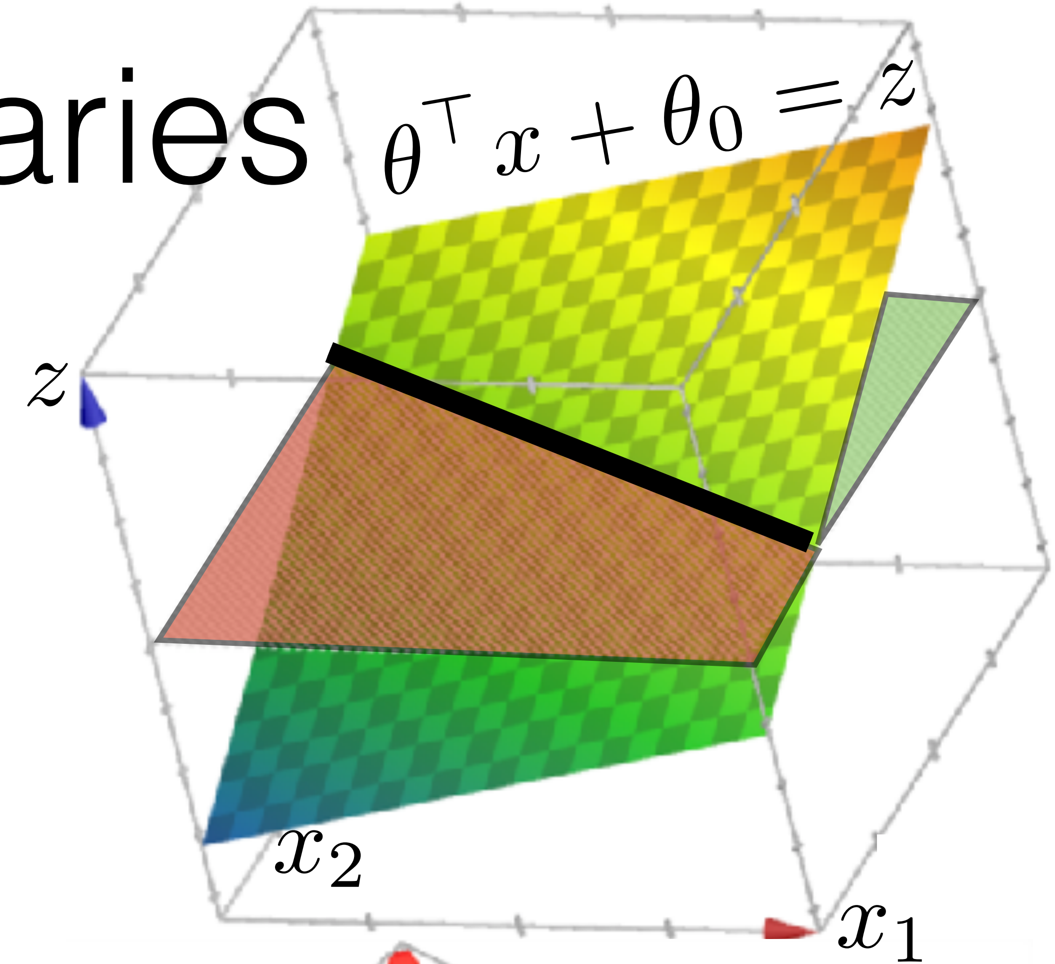

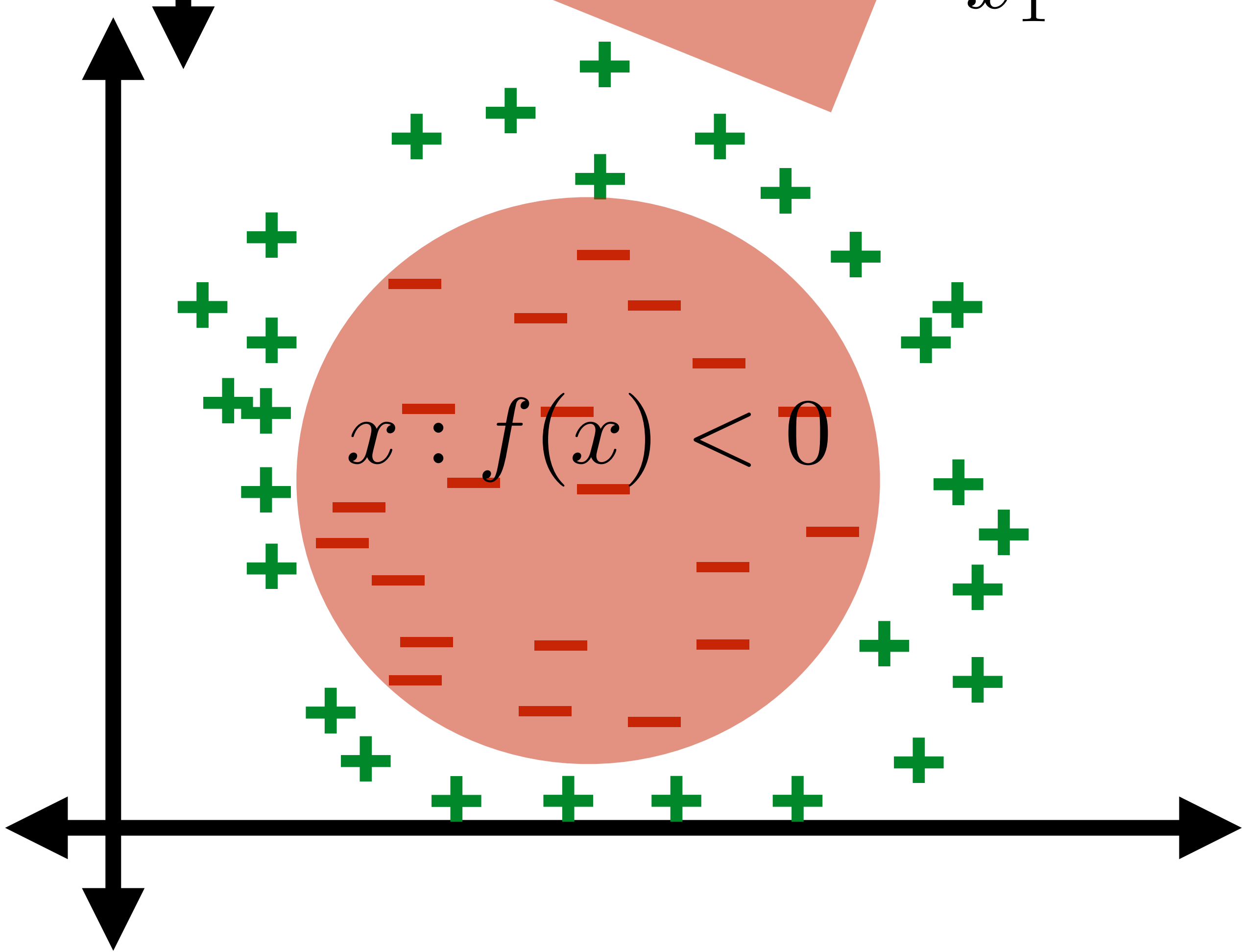

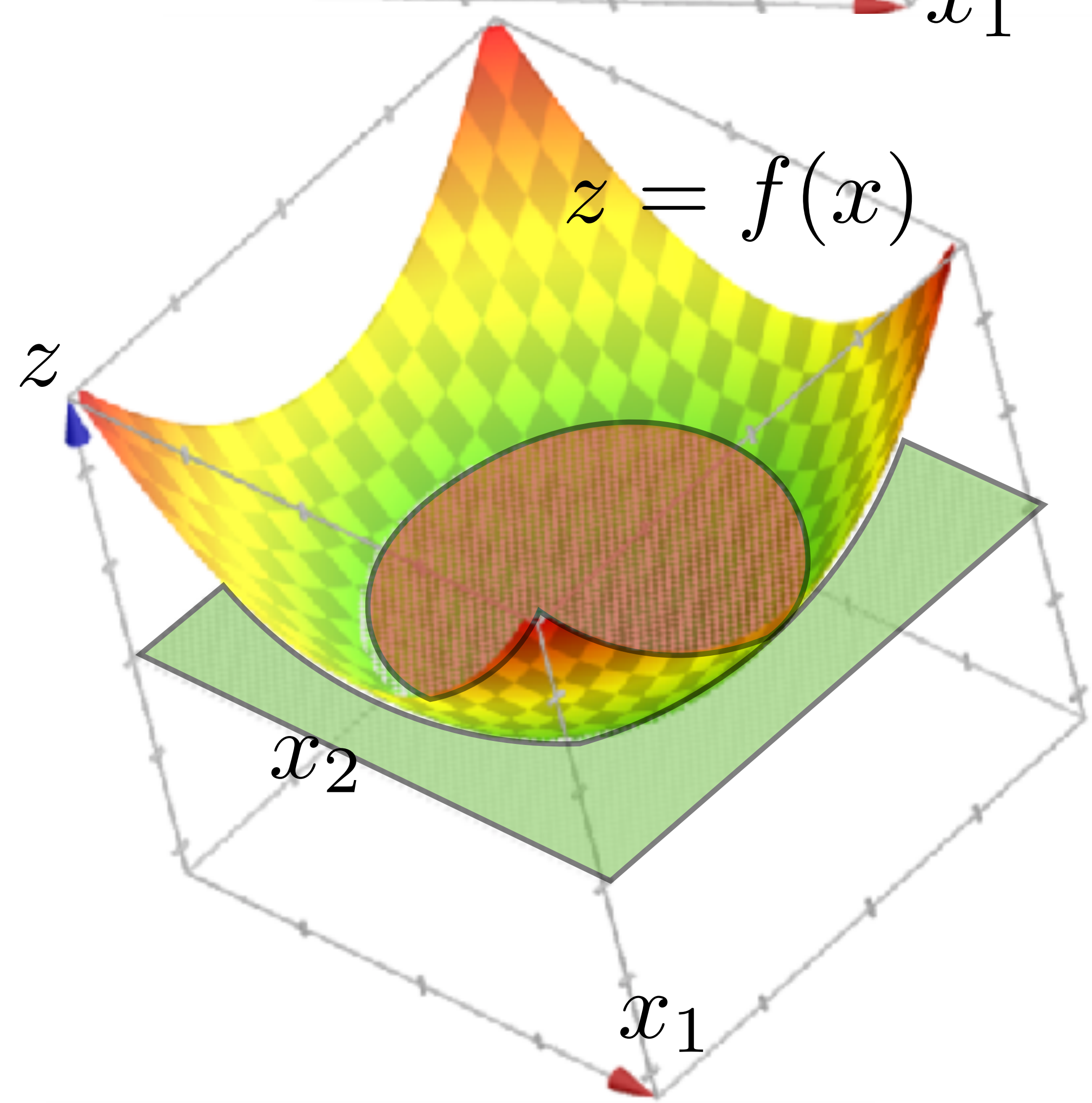

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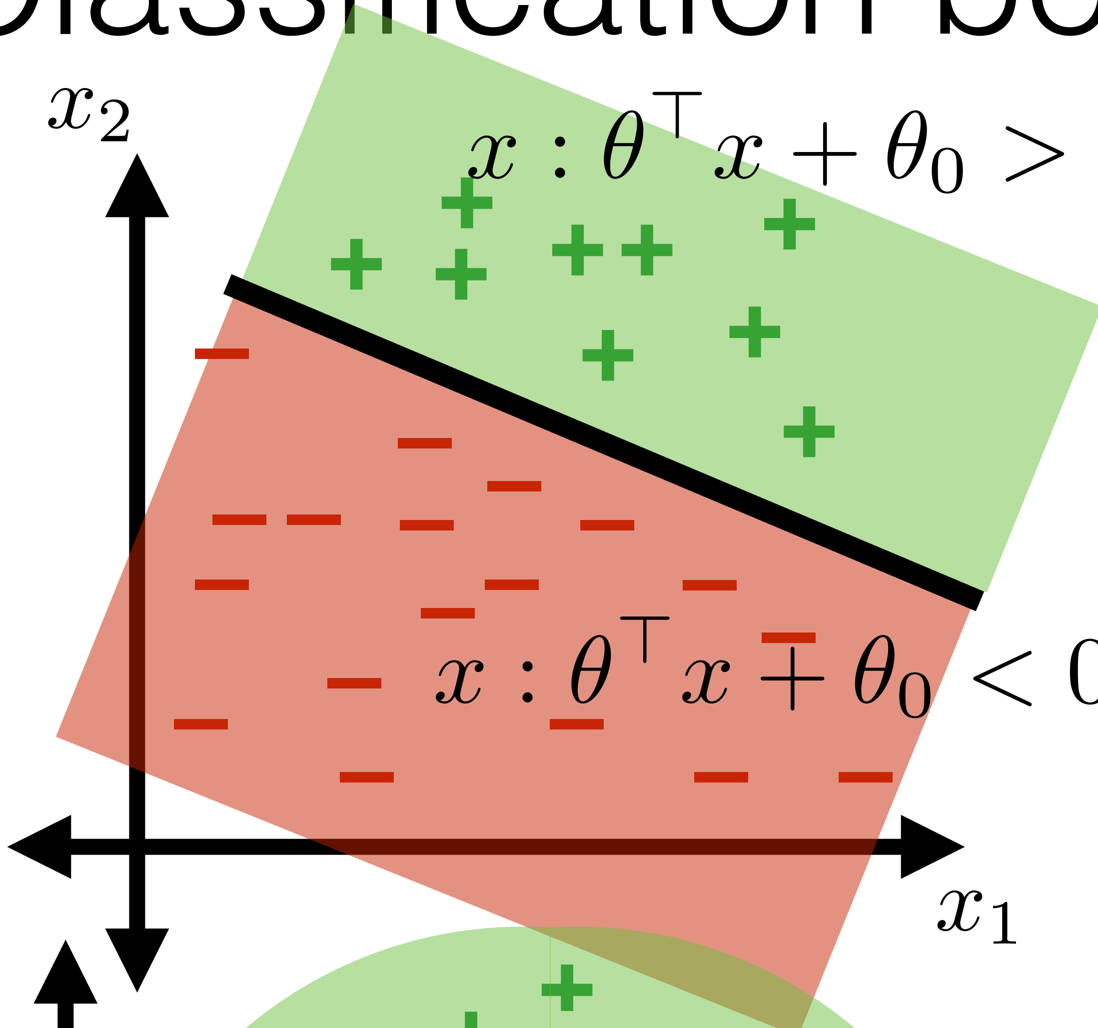

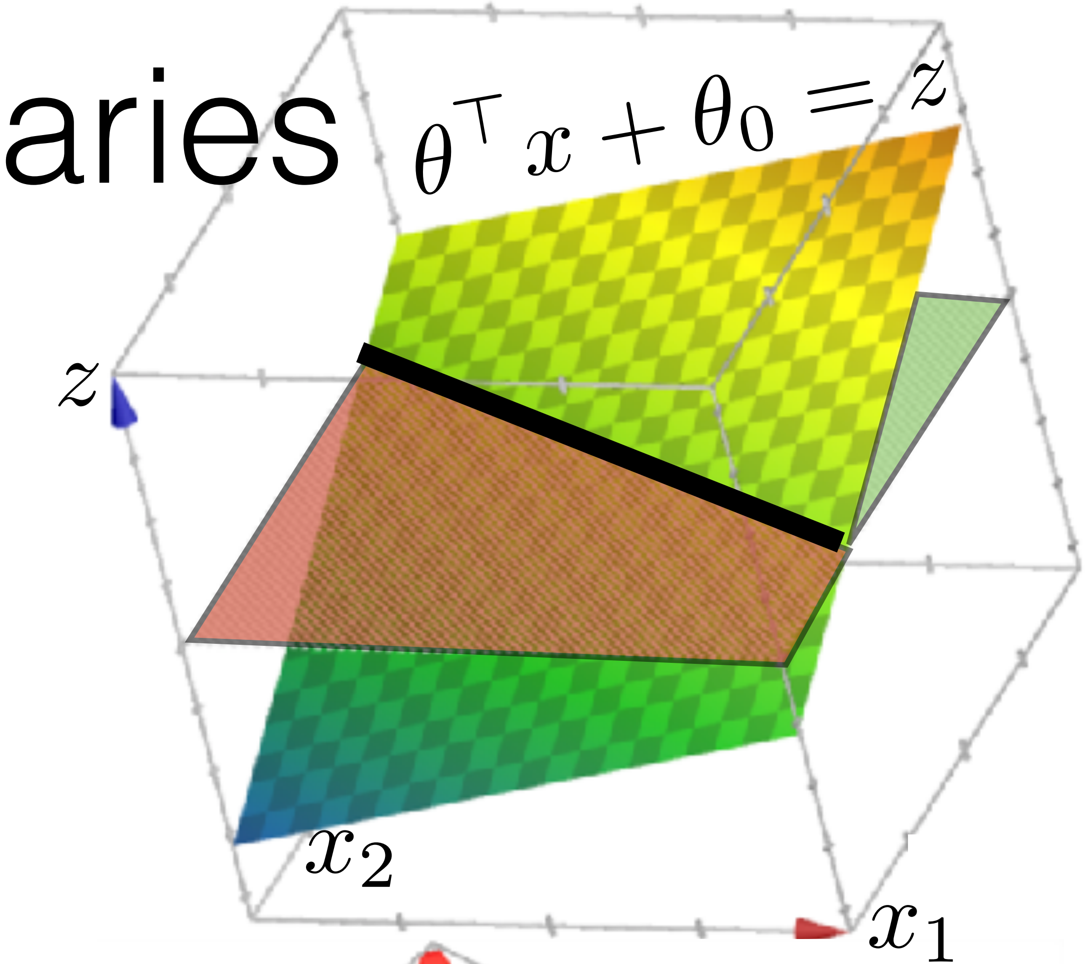

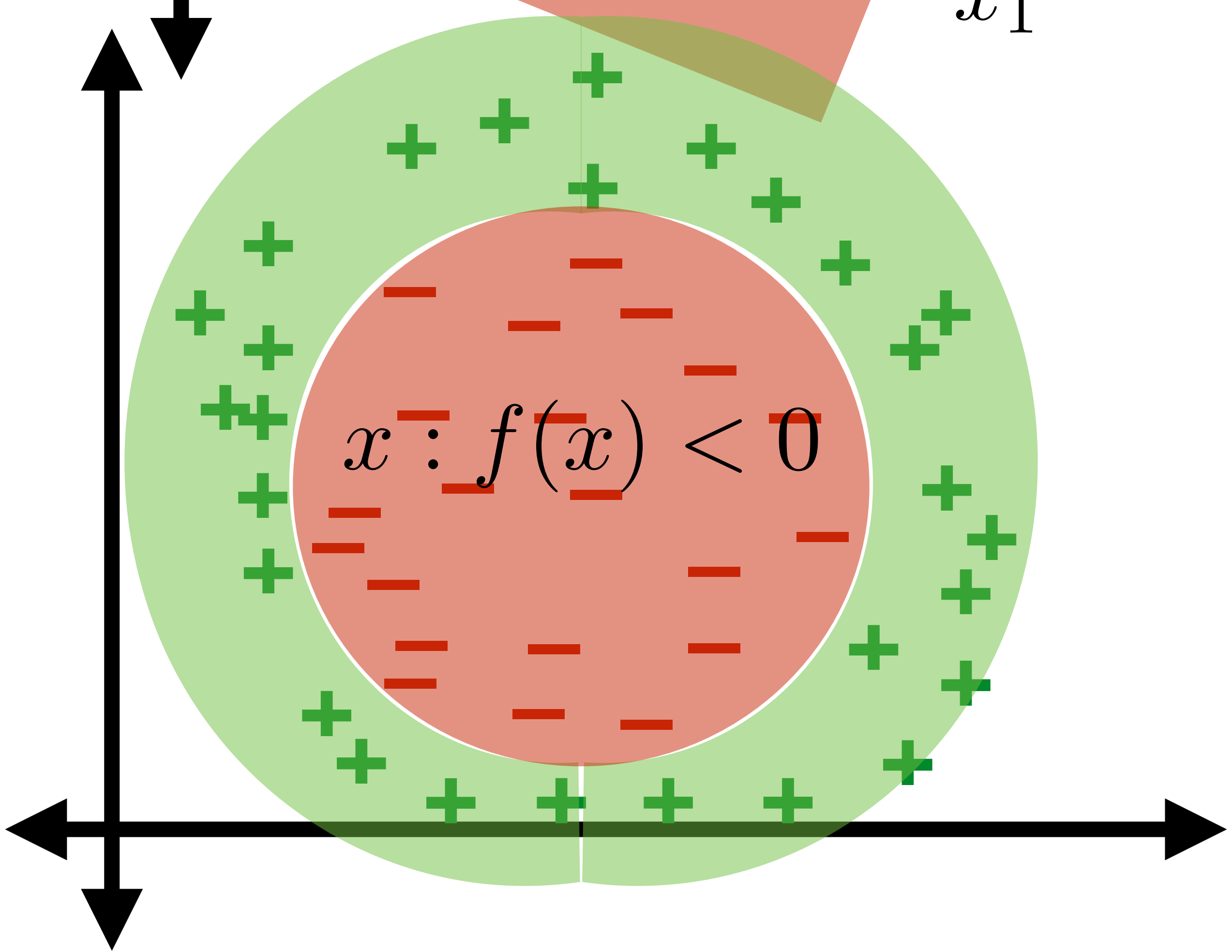

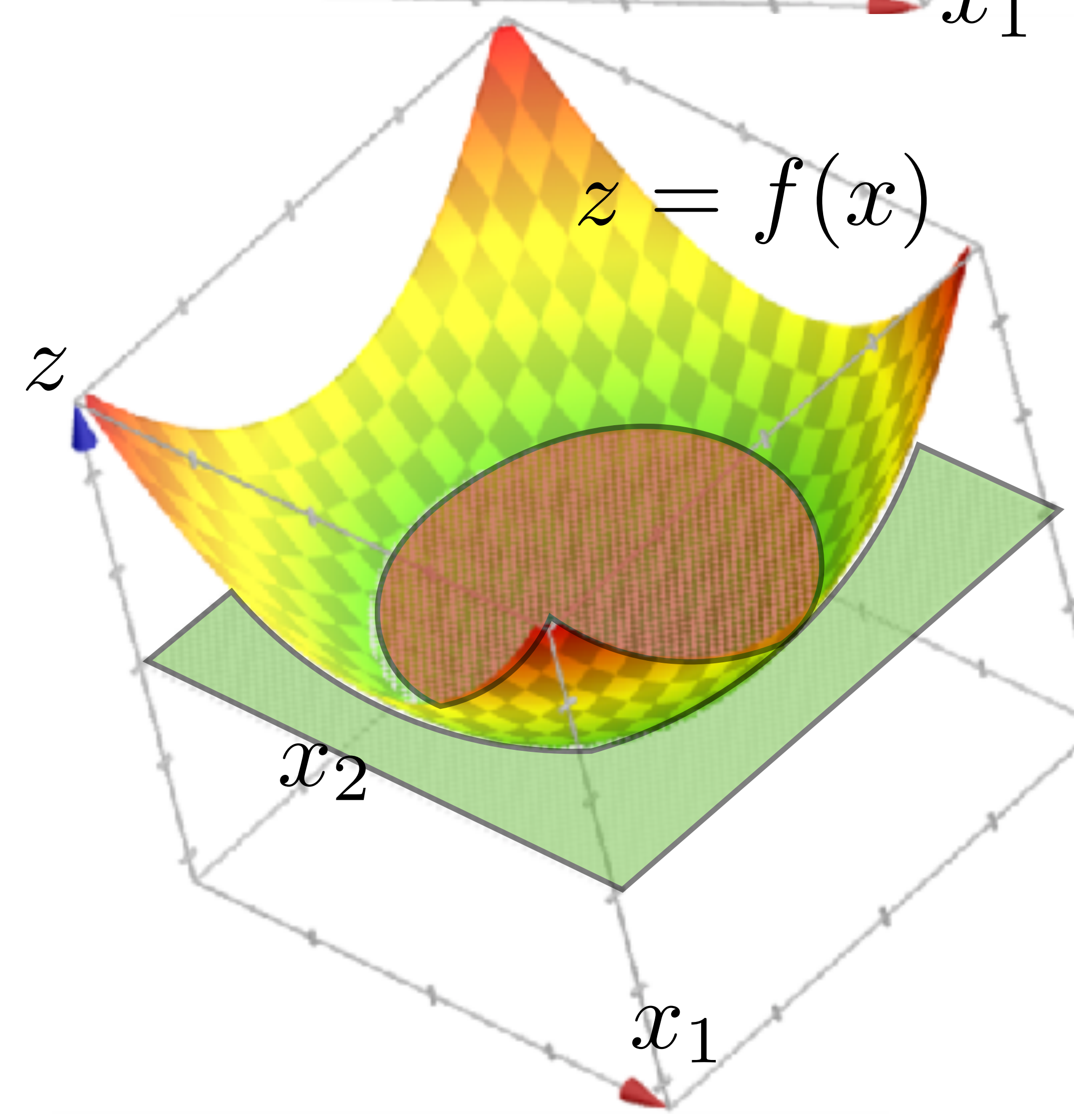

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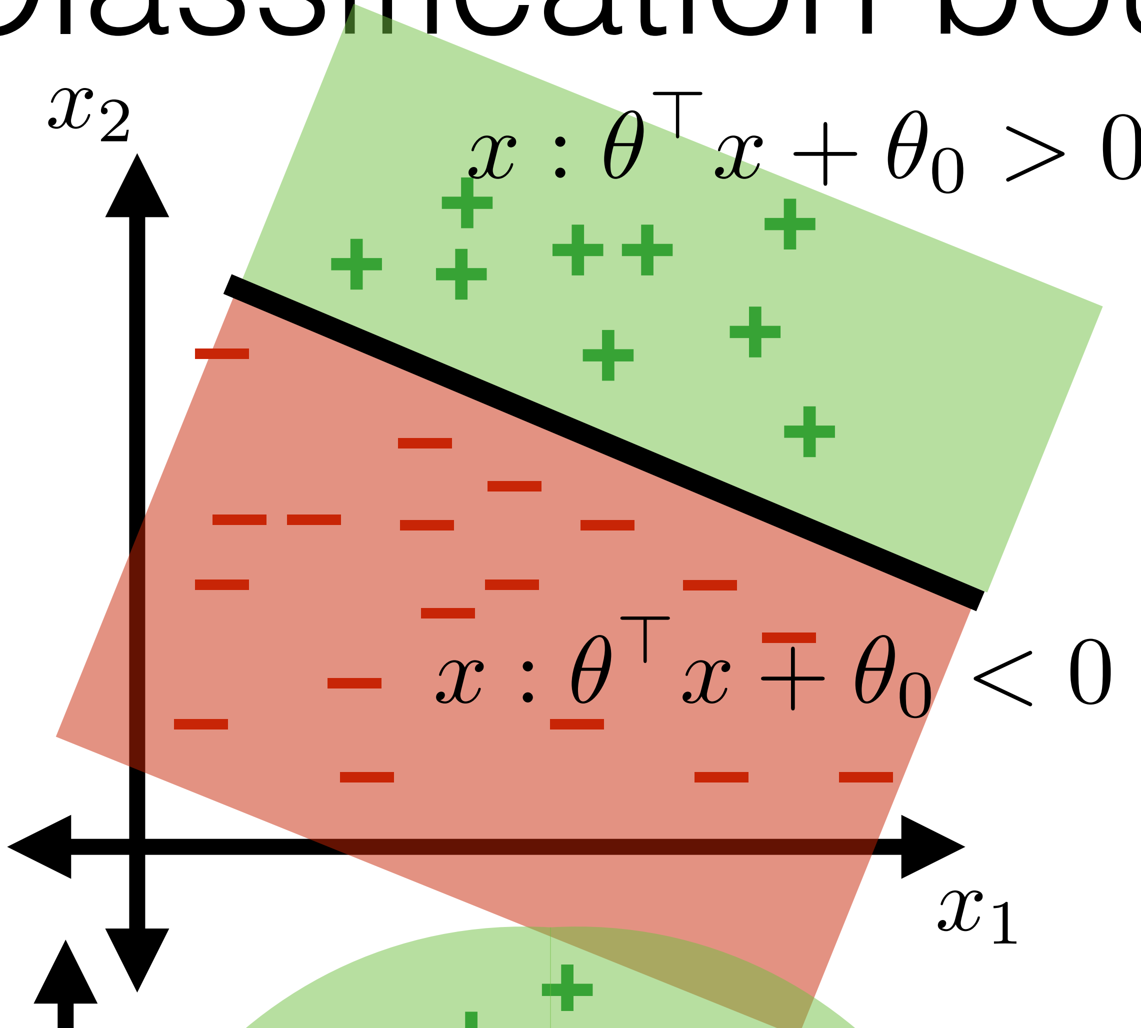

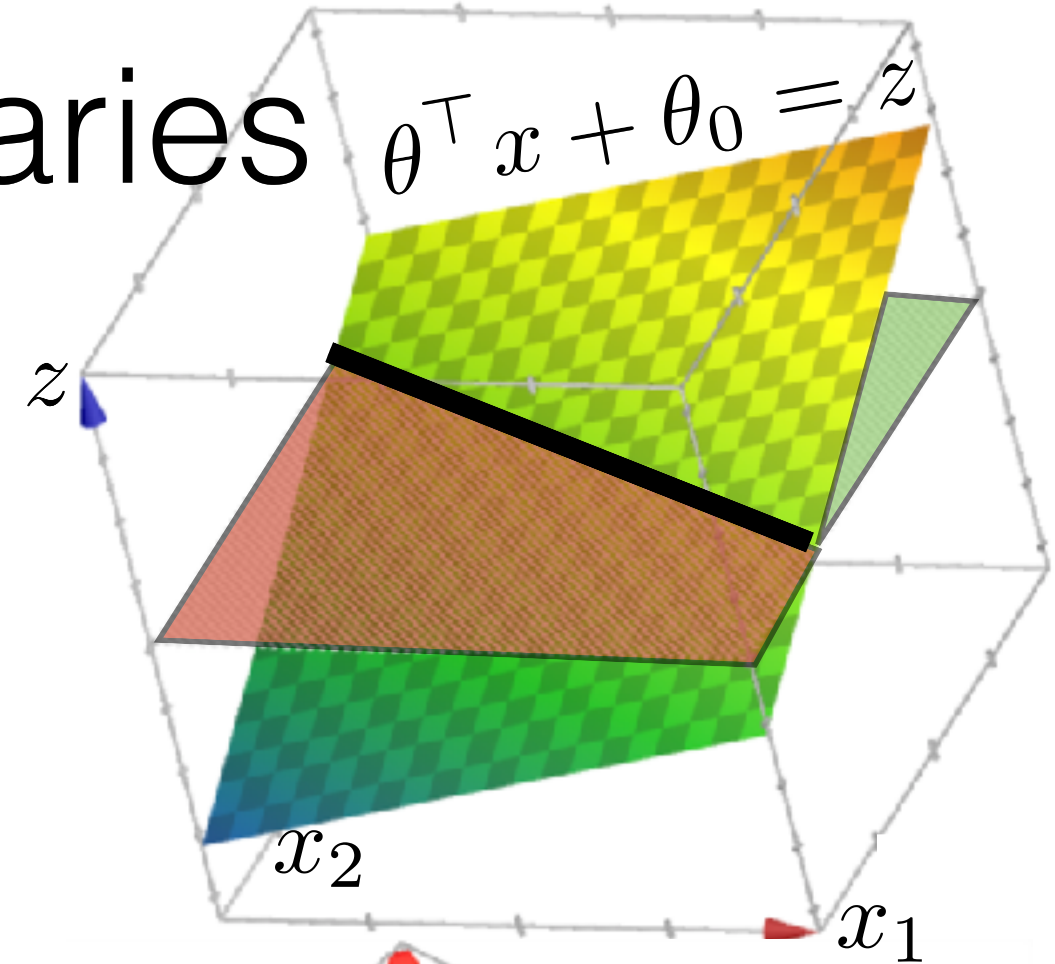

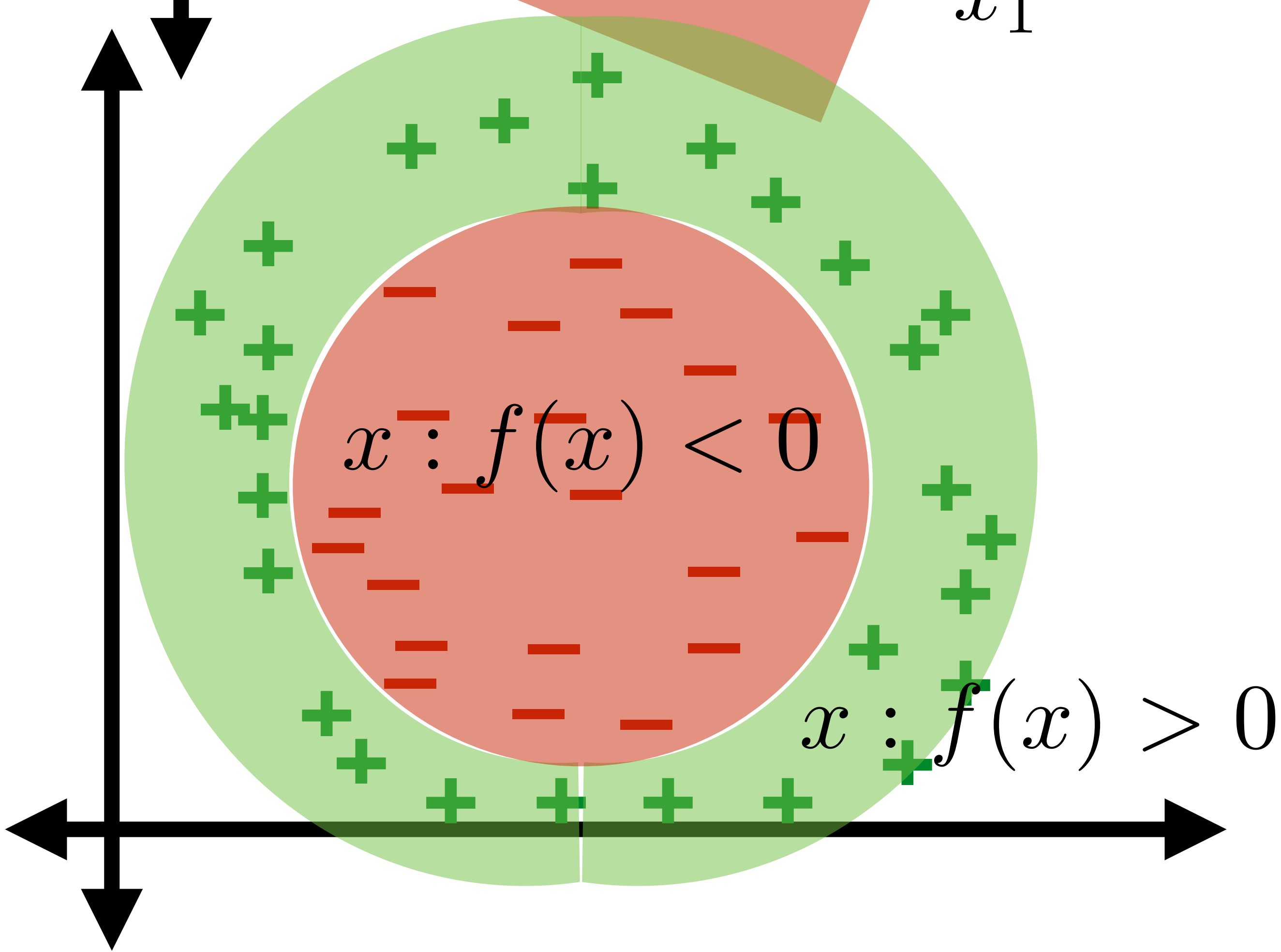

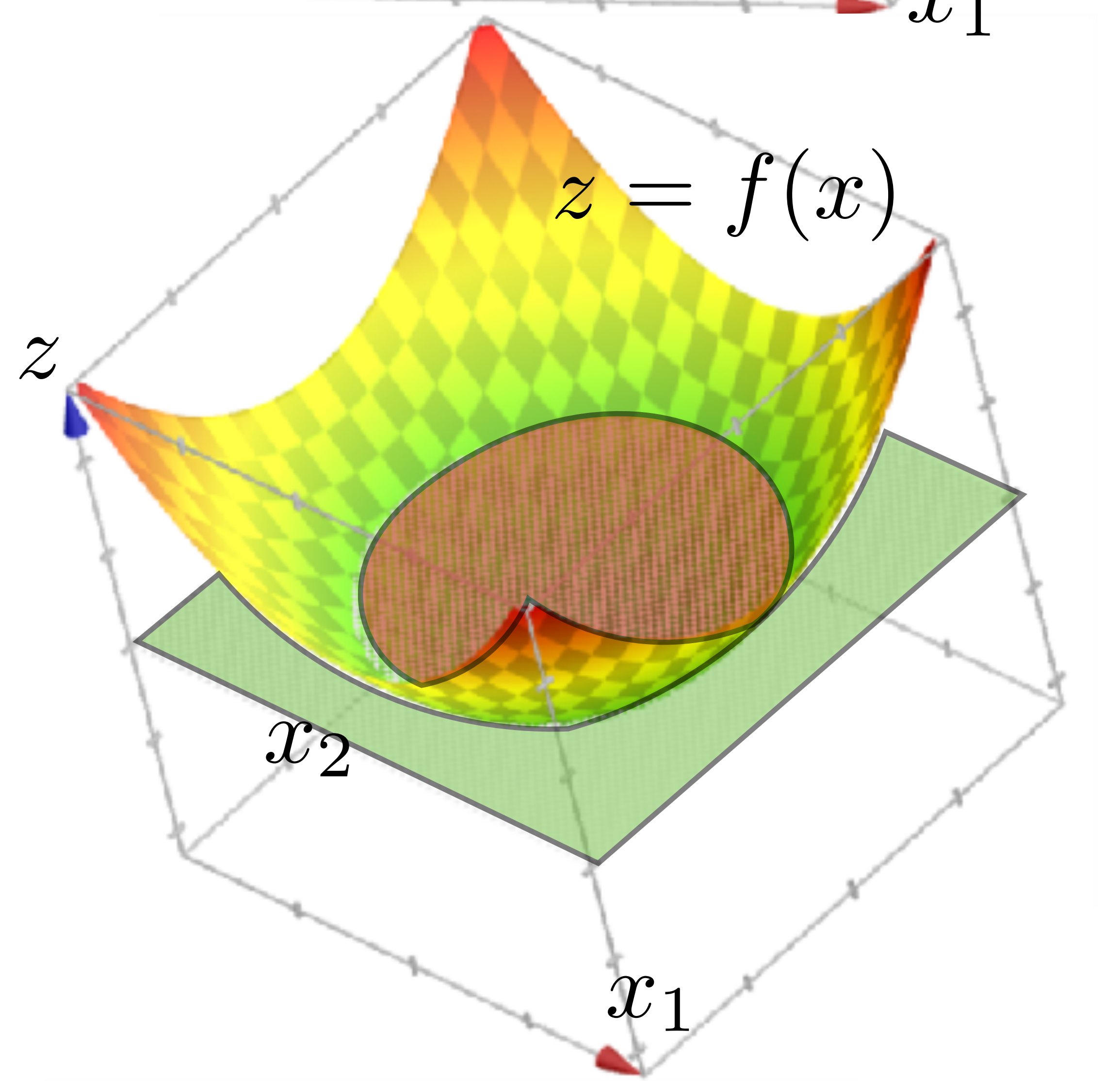

Nonlinear boundaries

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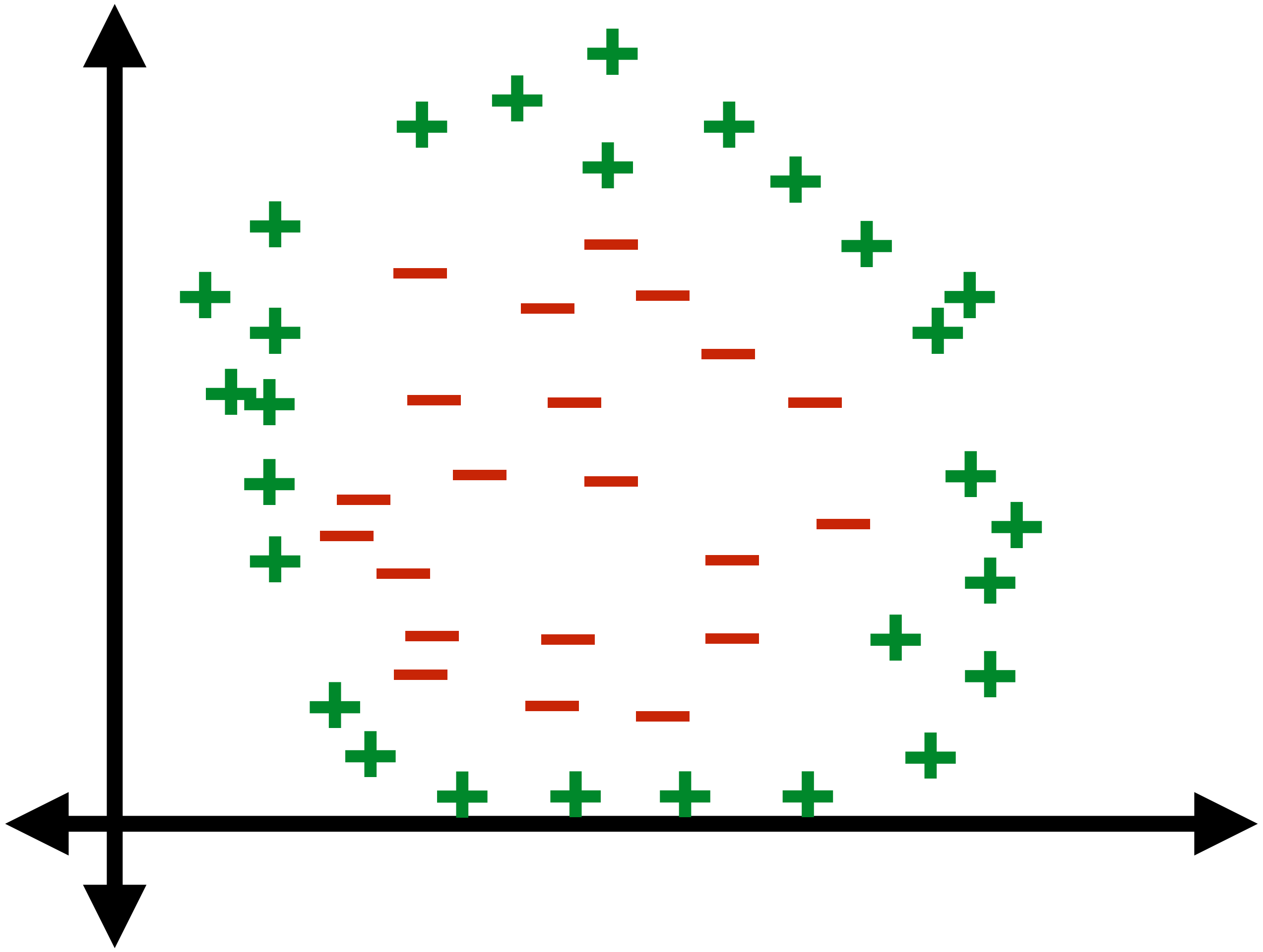

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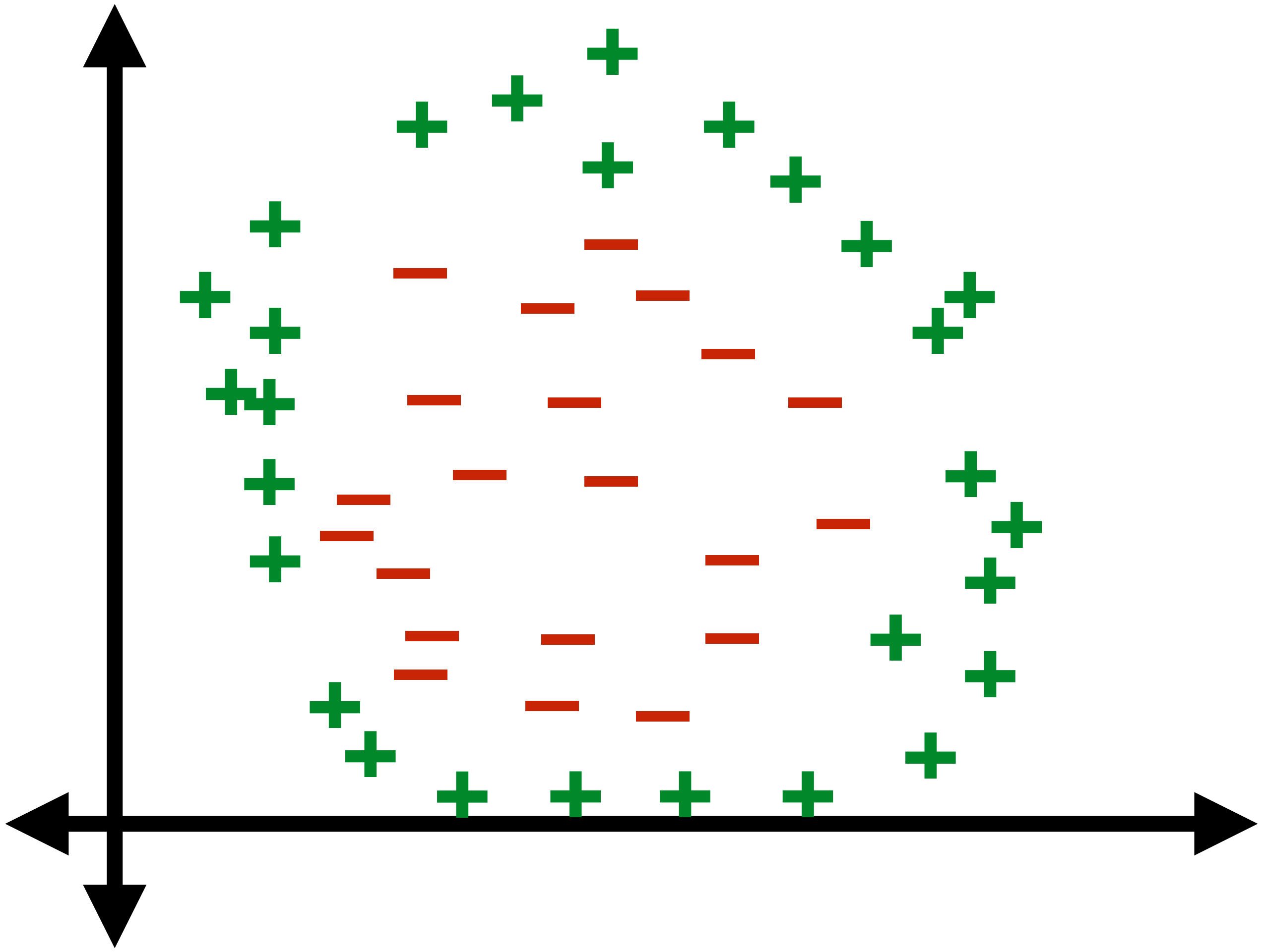

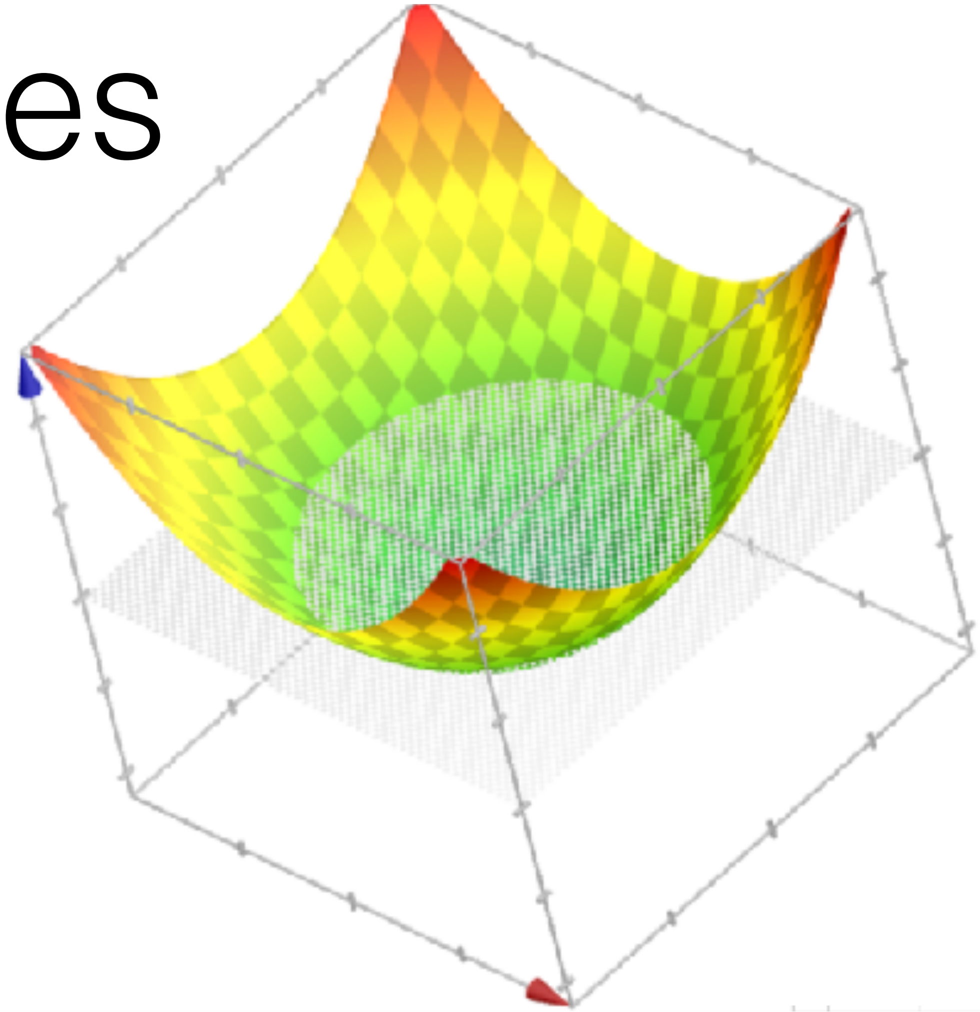

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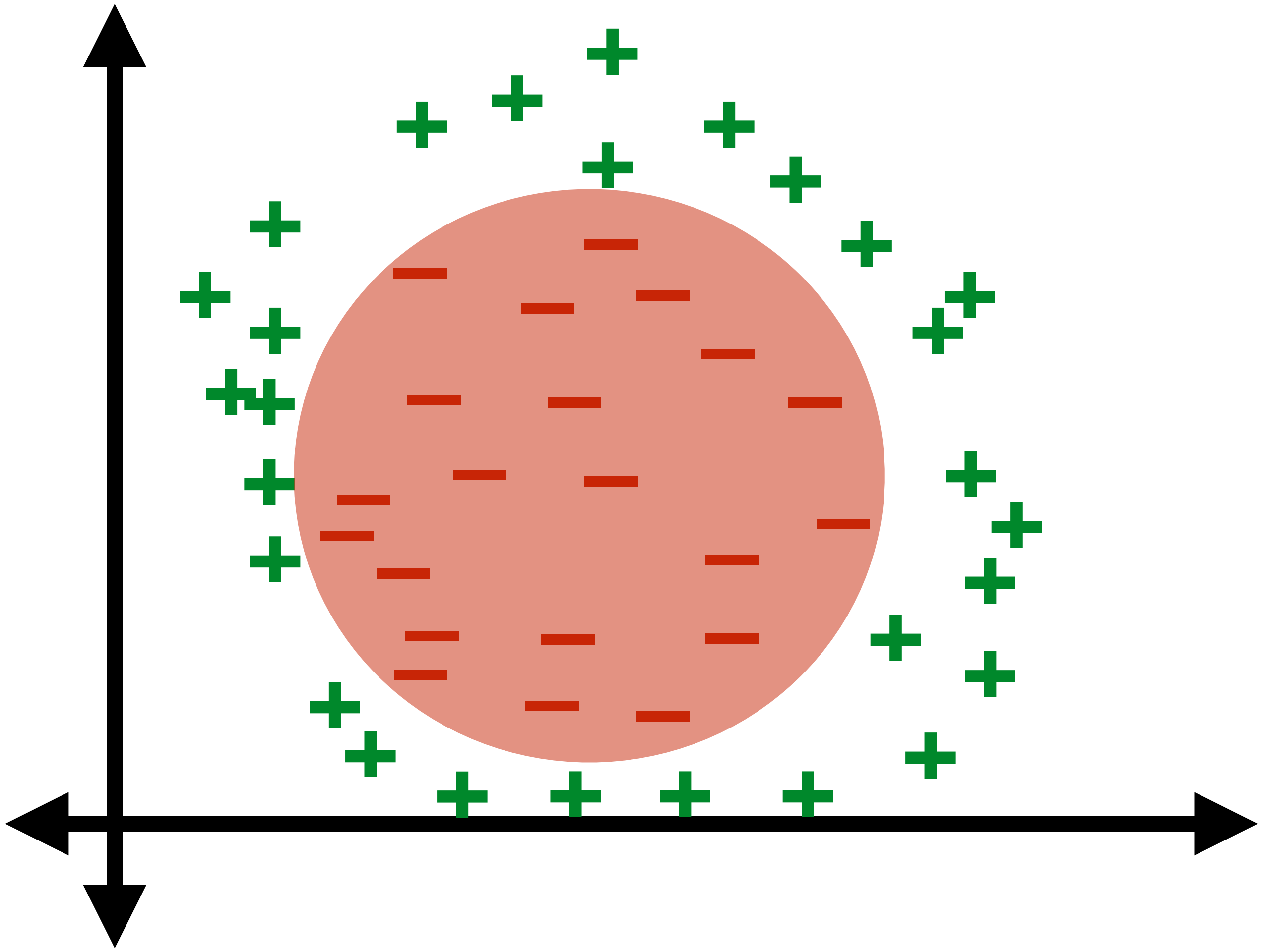

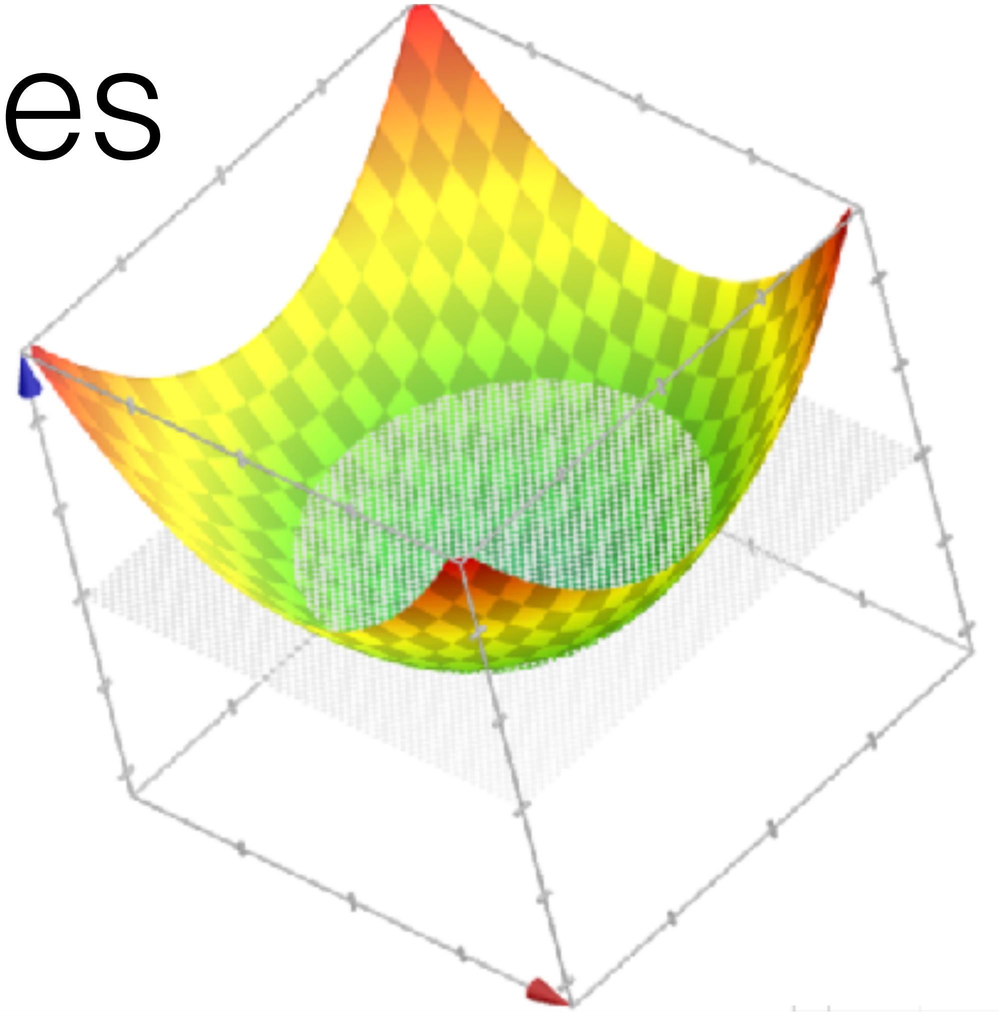

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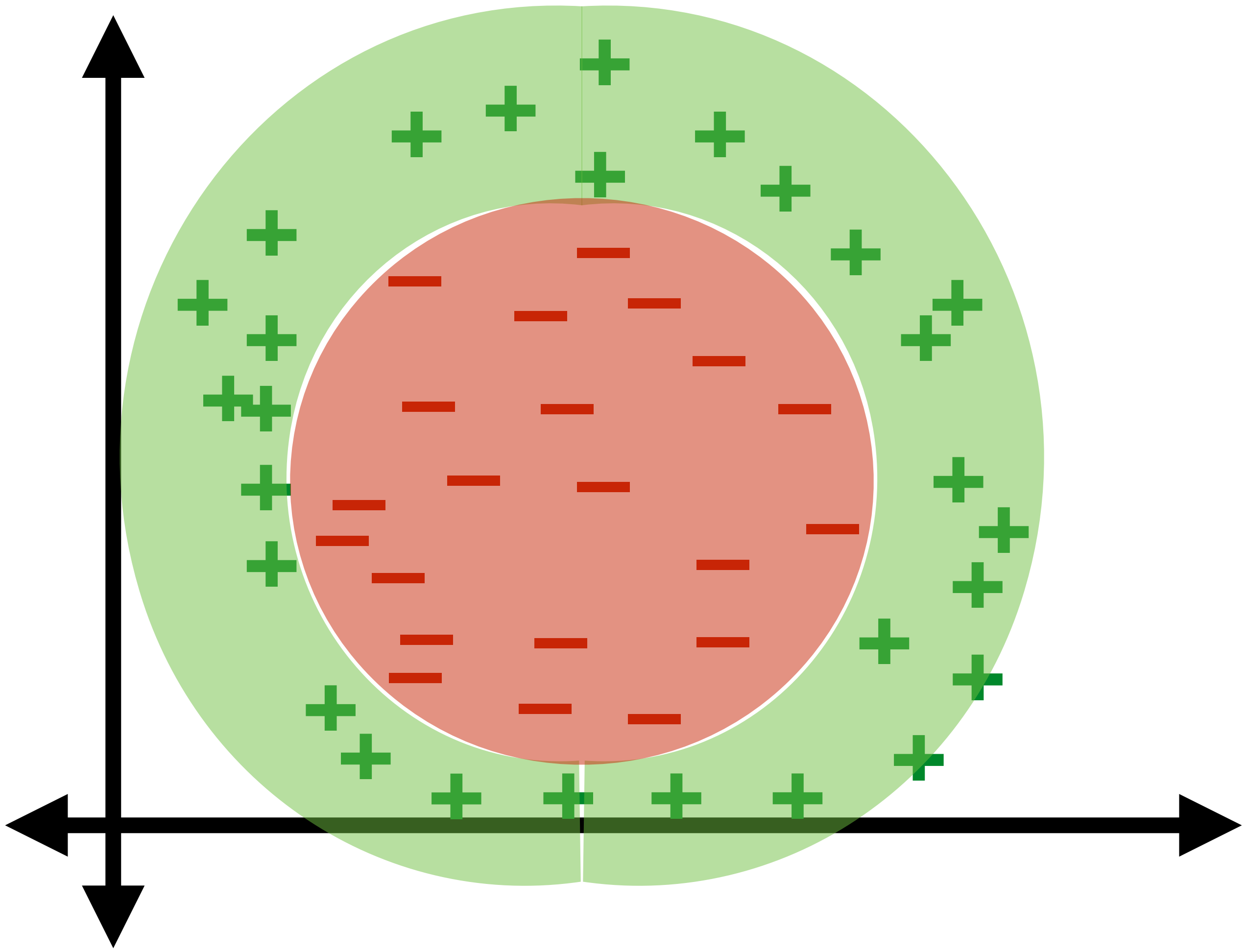

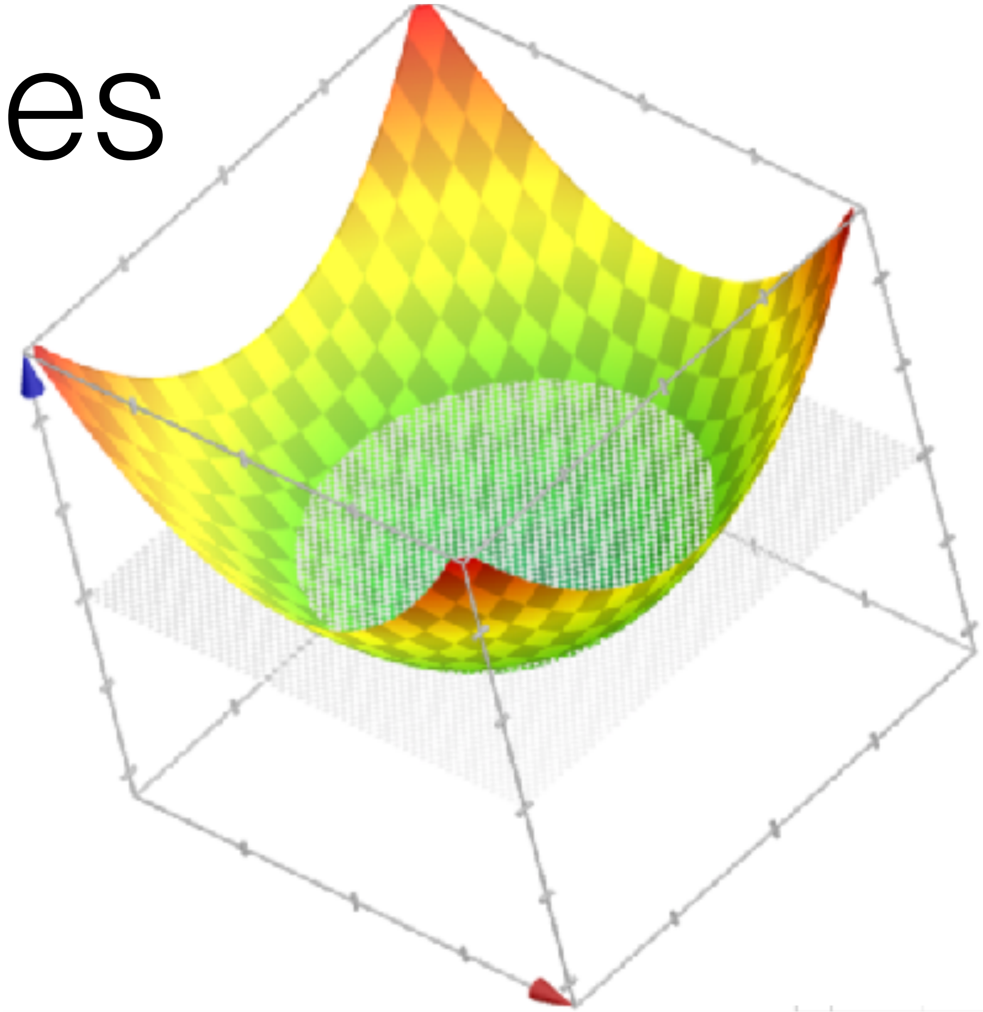

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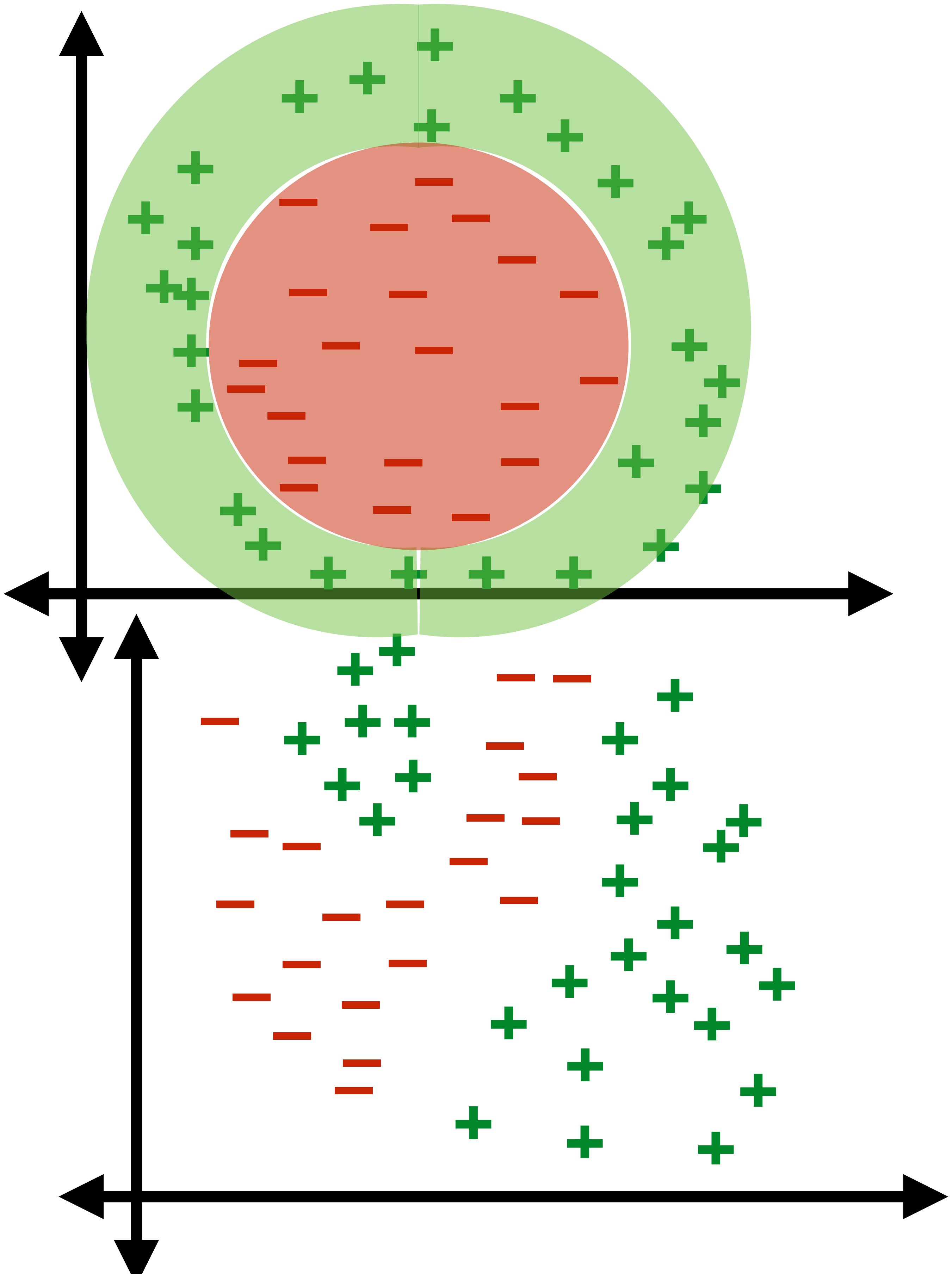

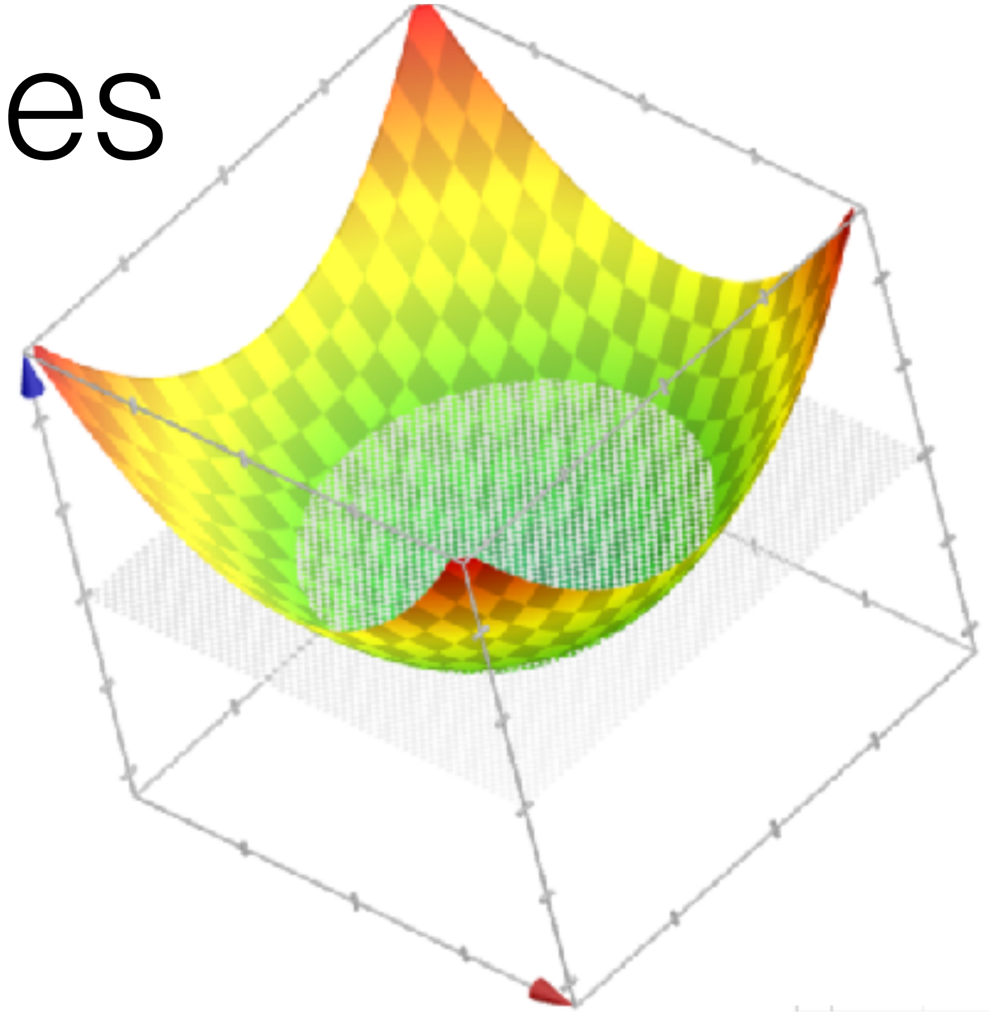

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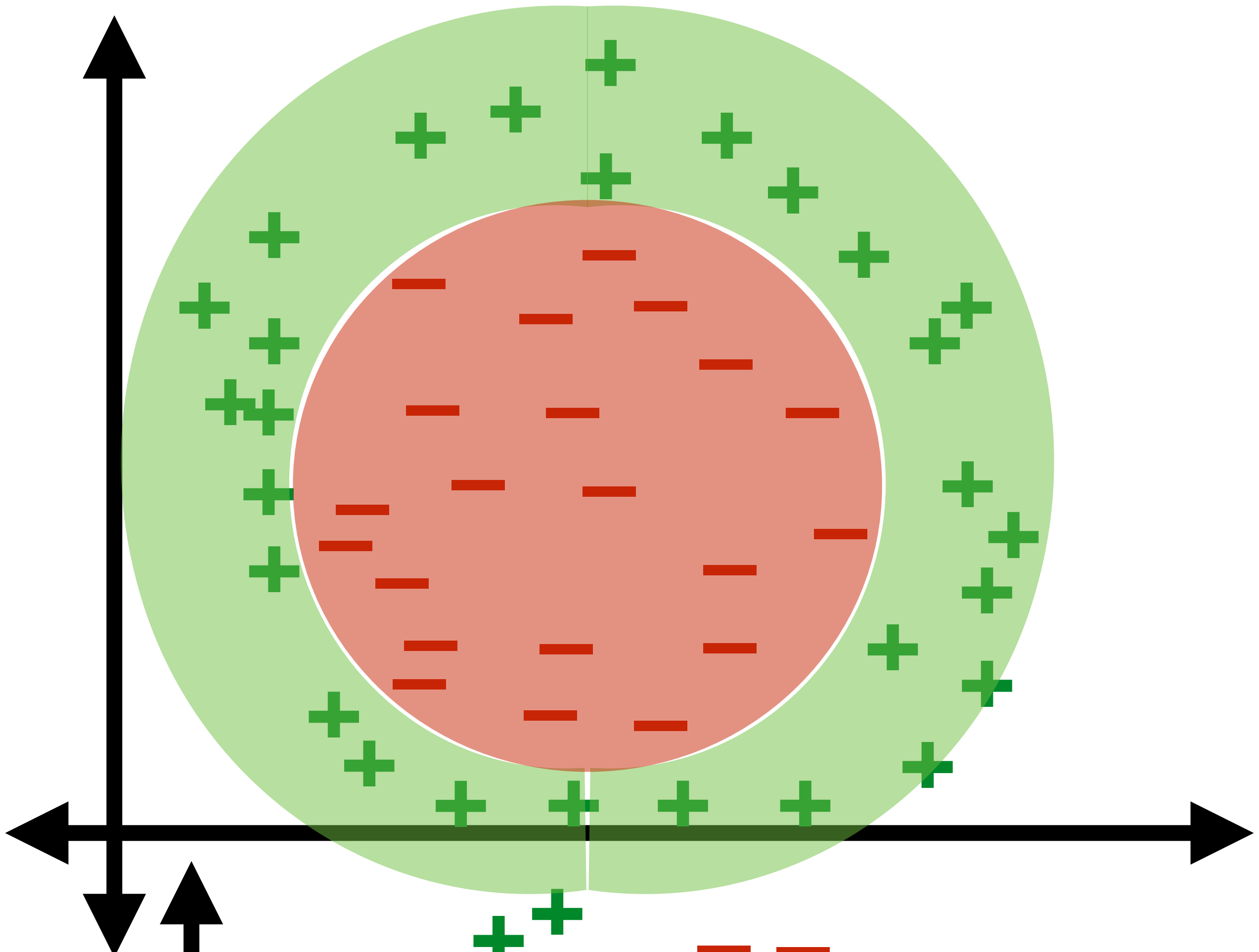

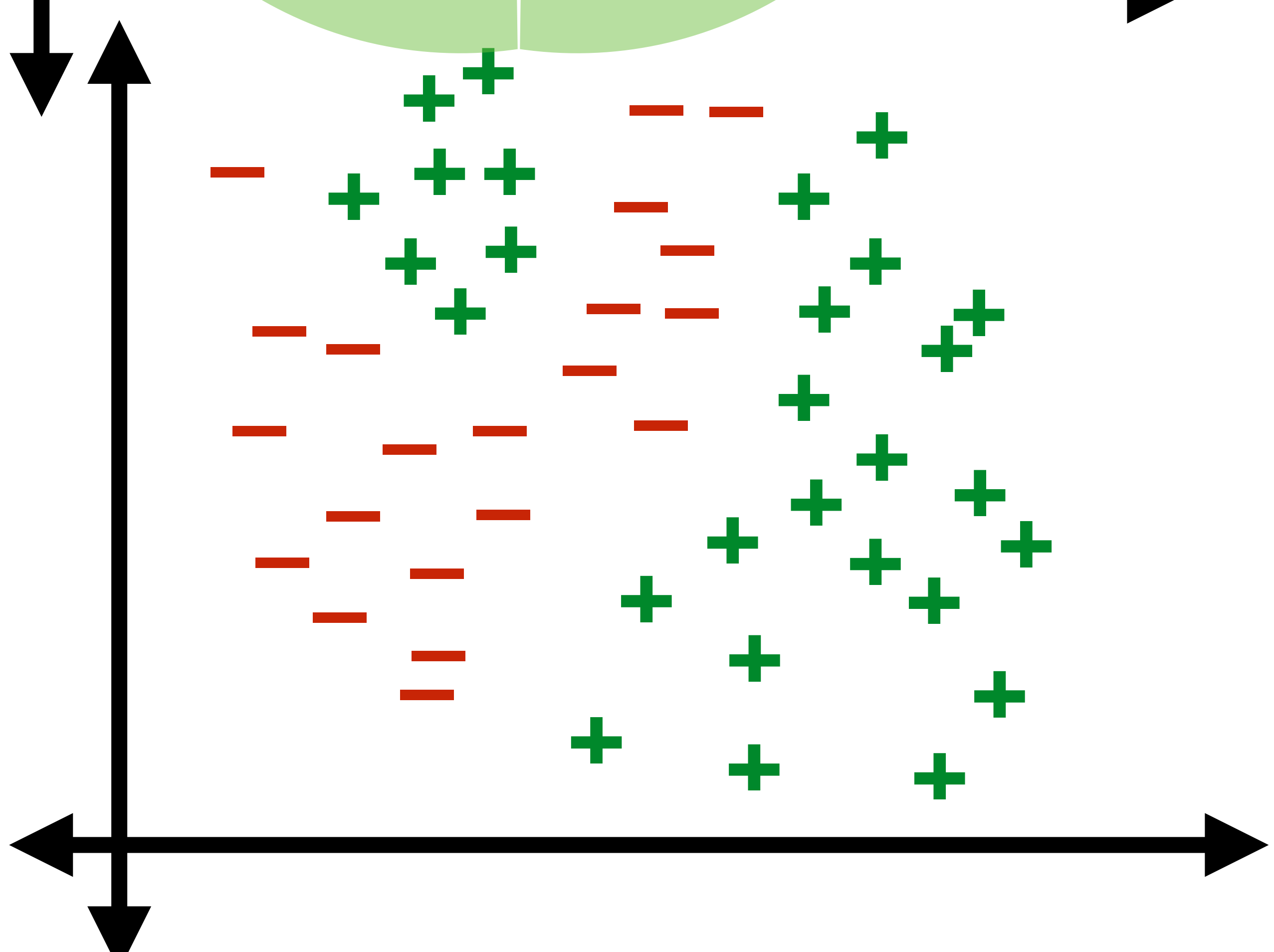

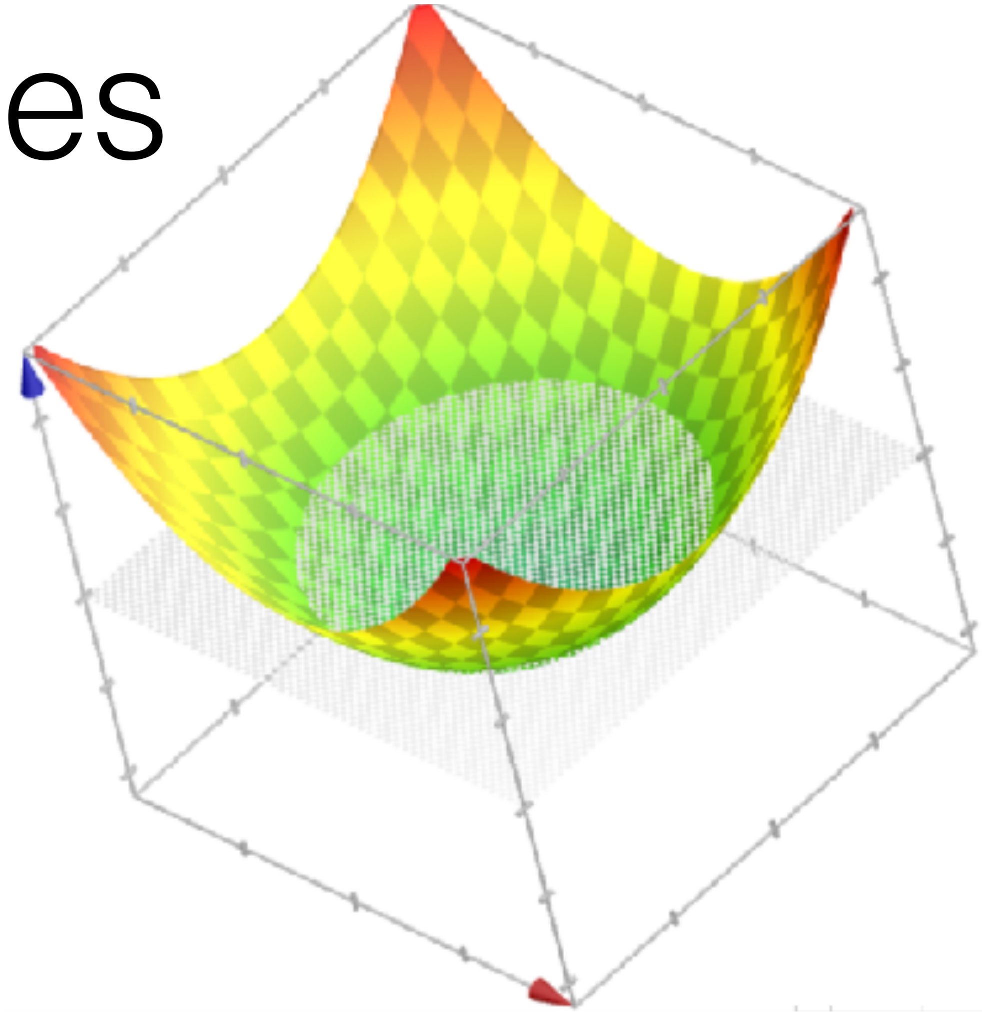

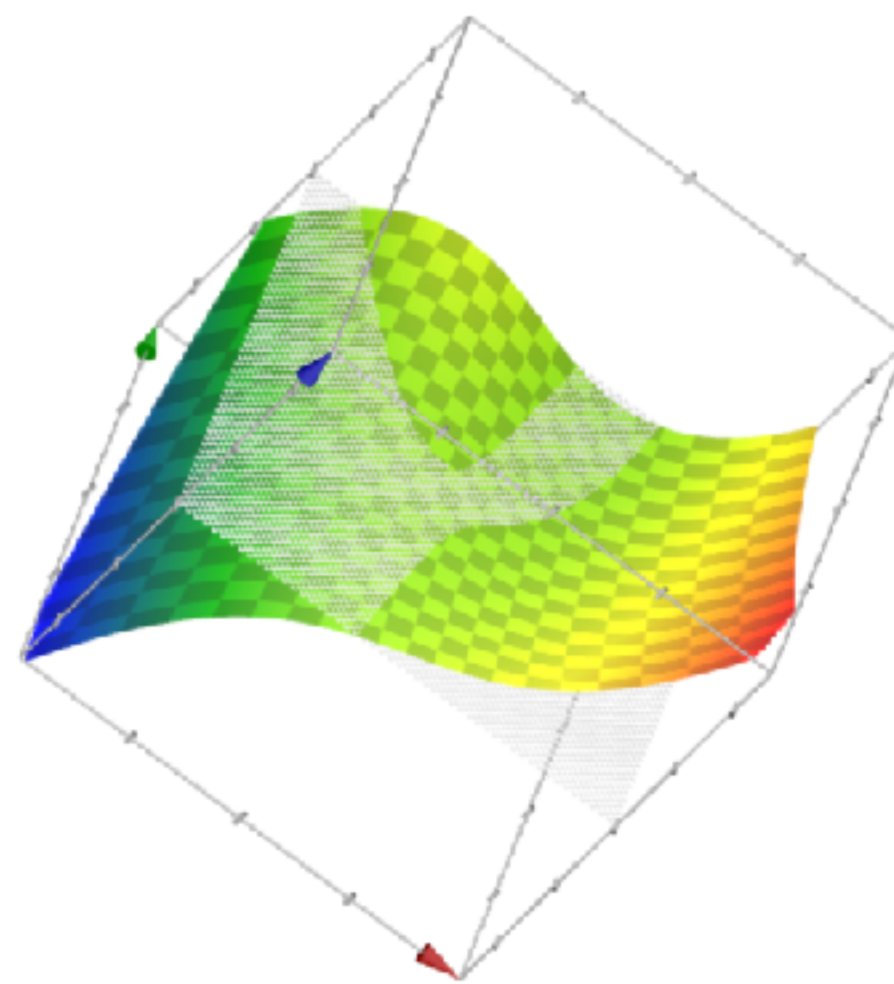

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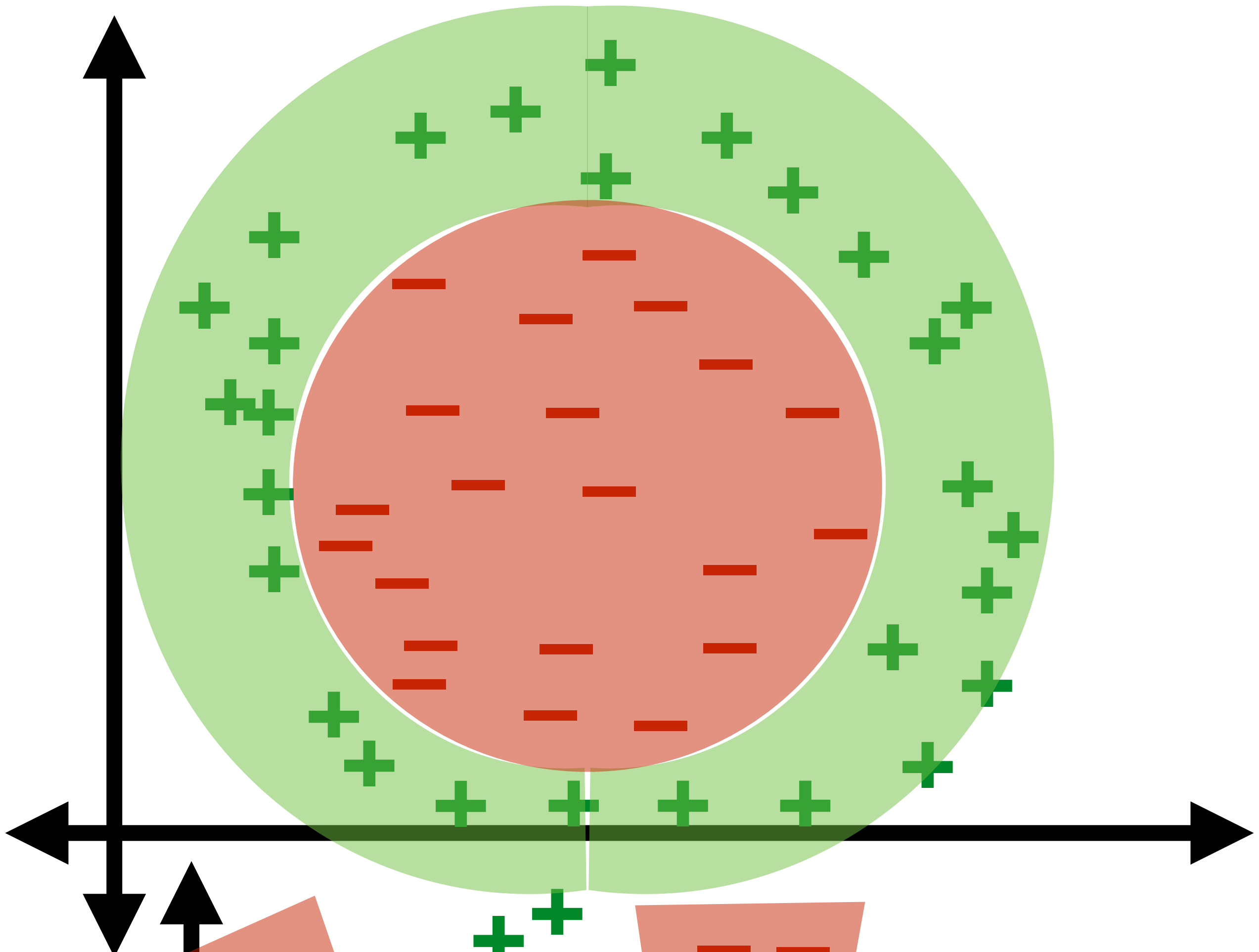
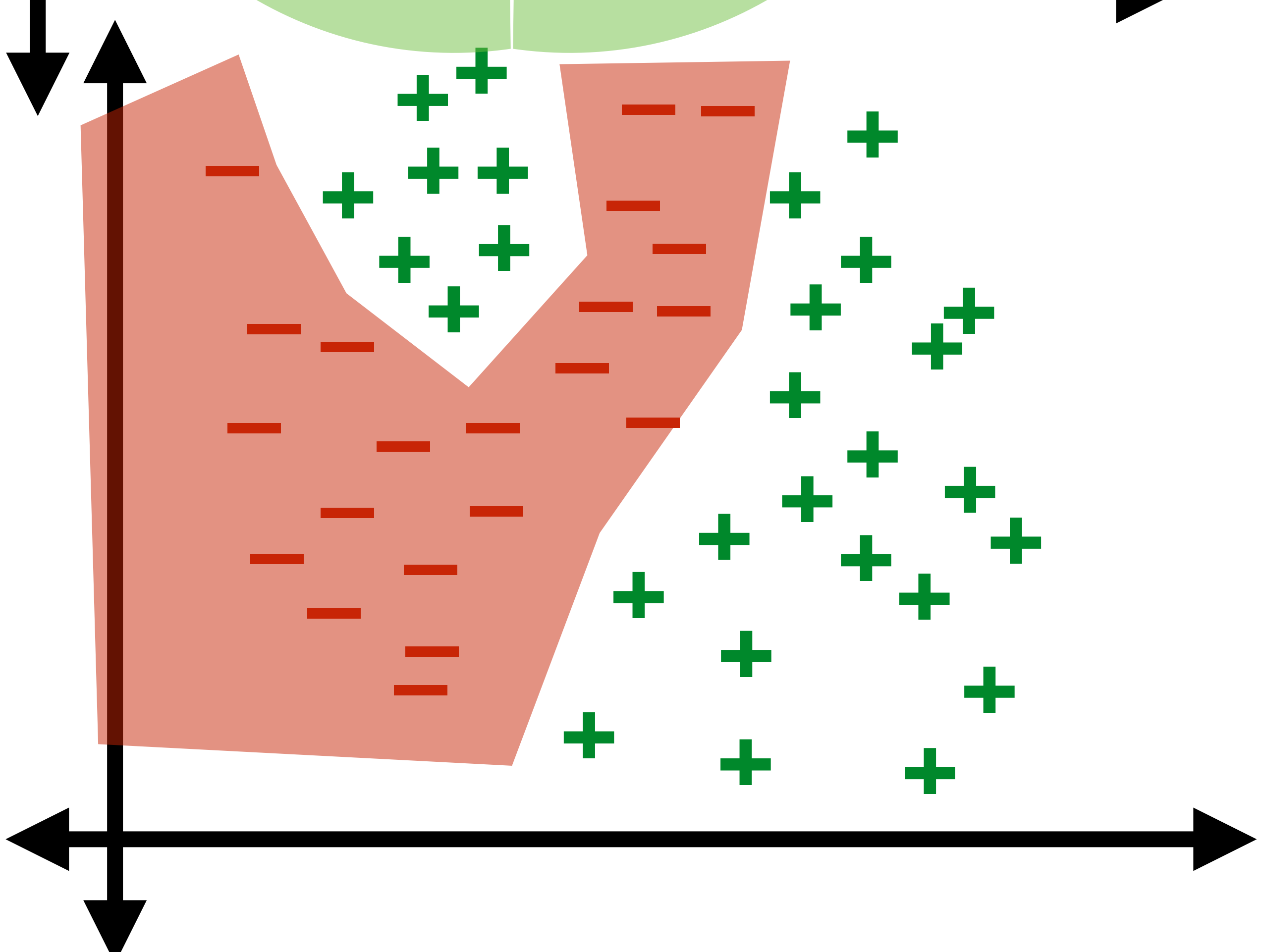
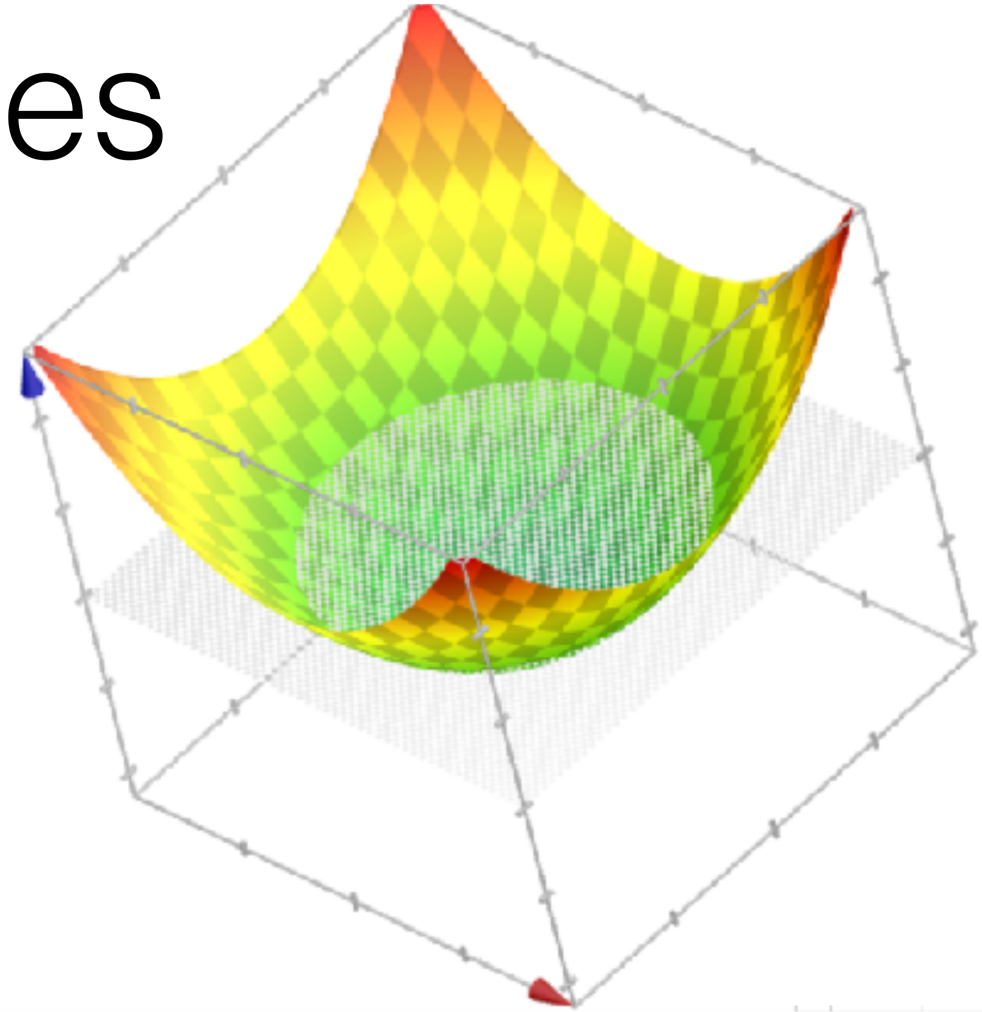
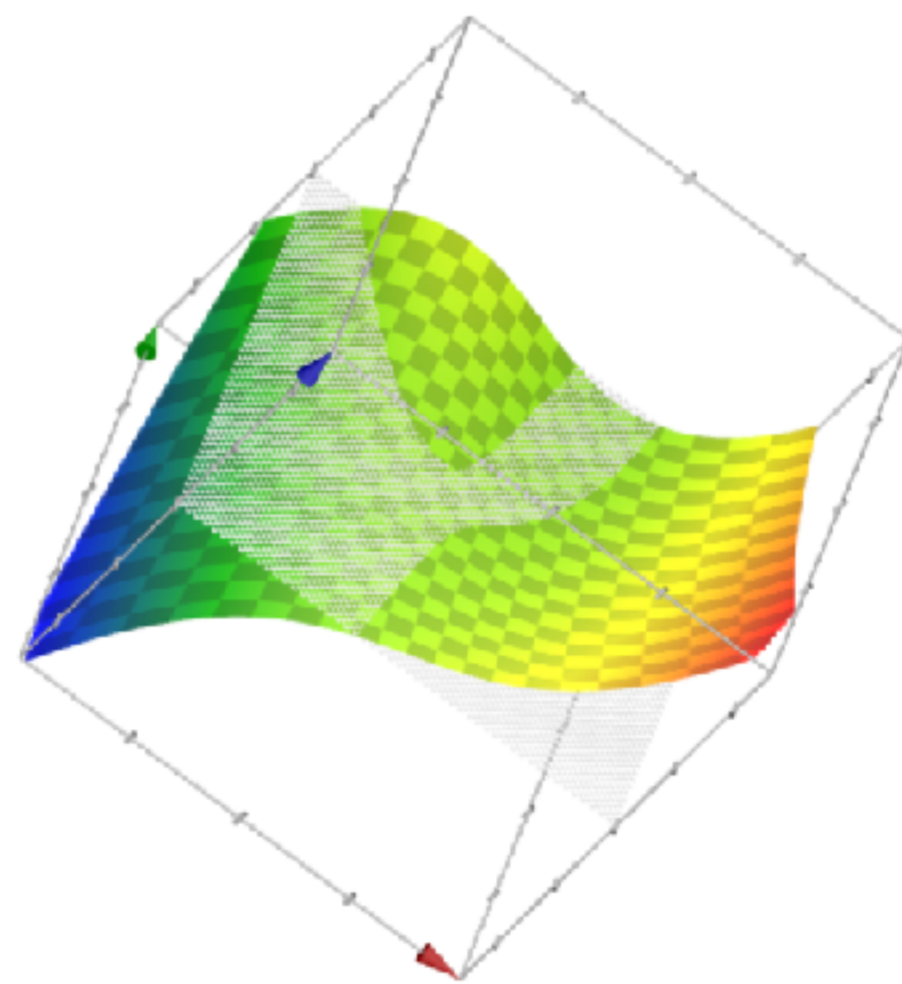
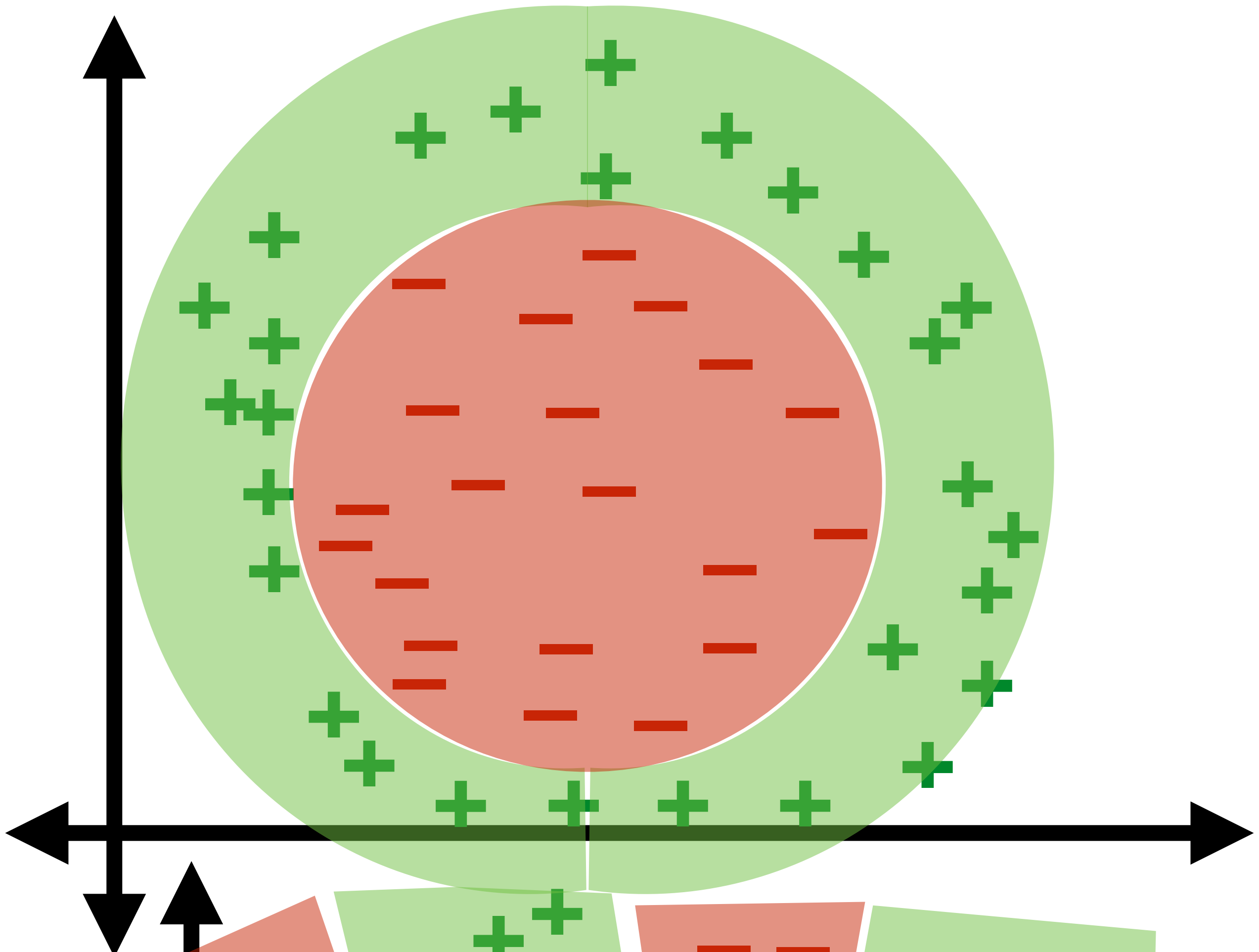


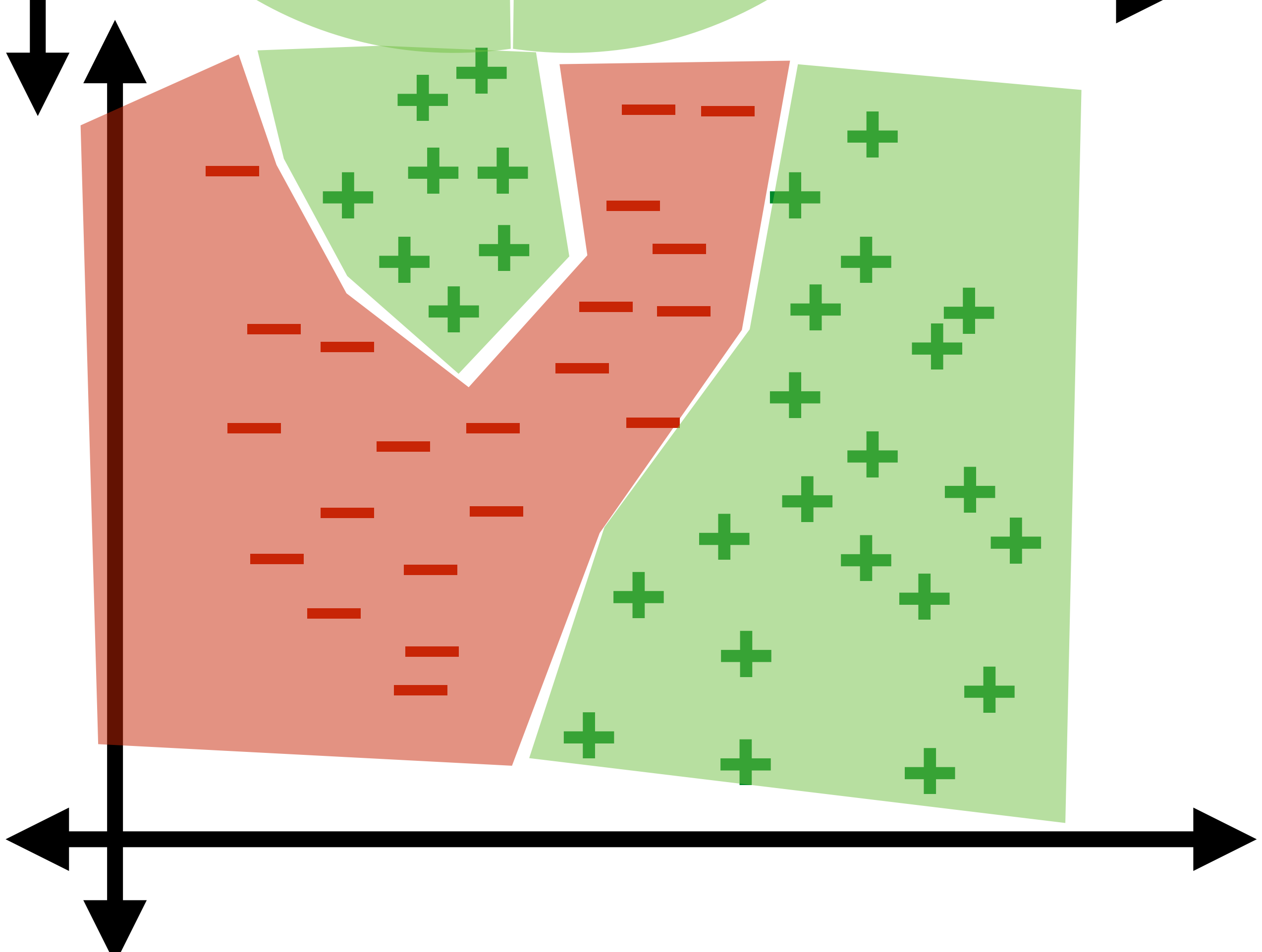


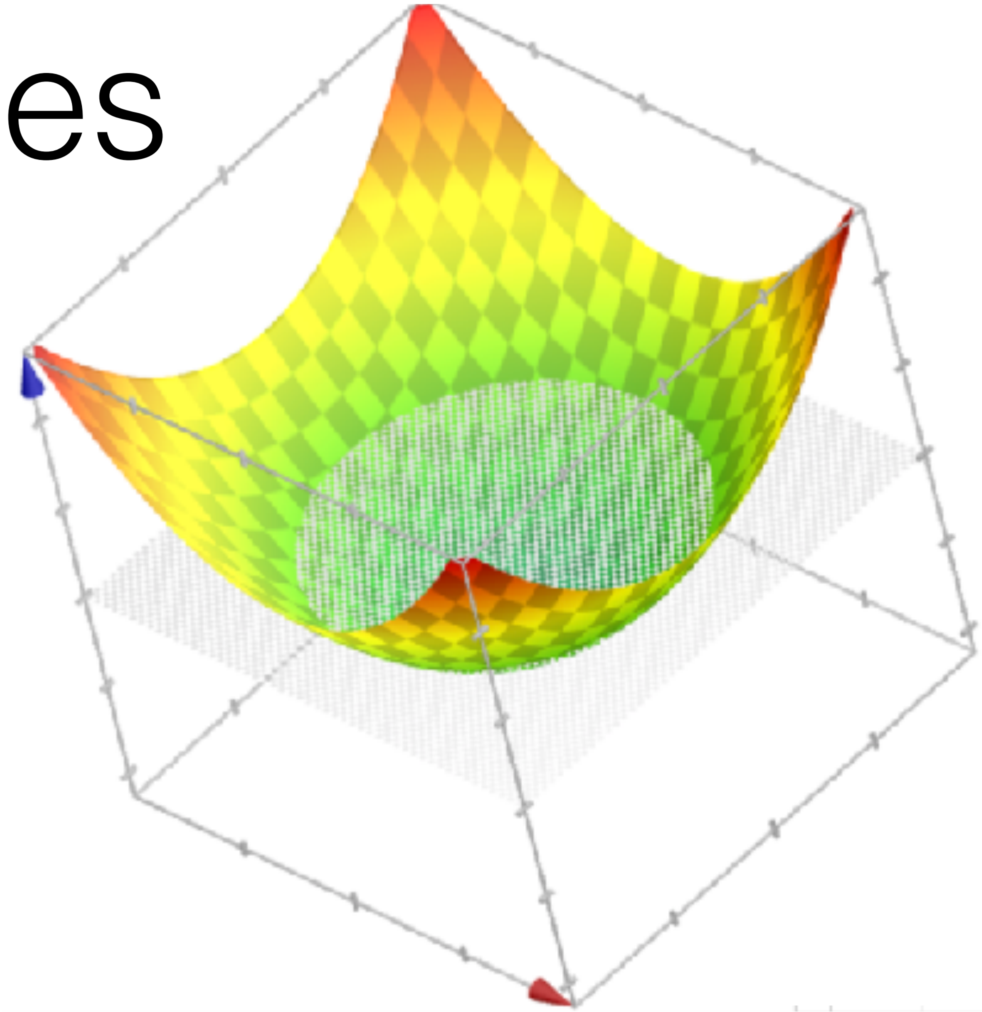


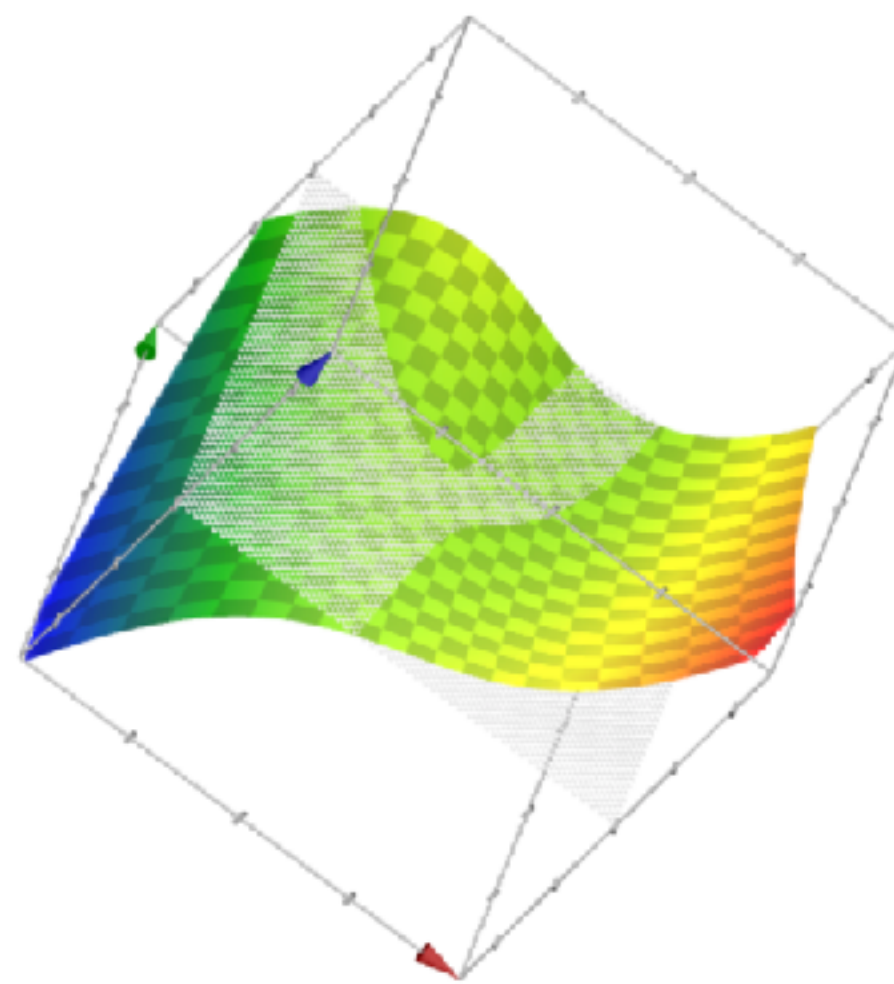


Nonlinear boundaries









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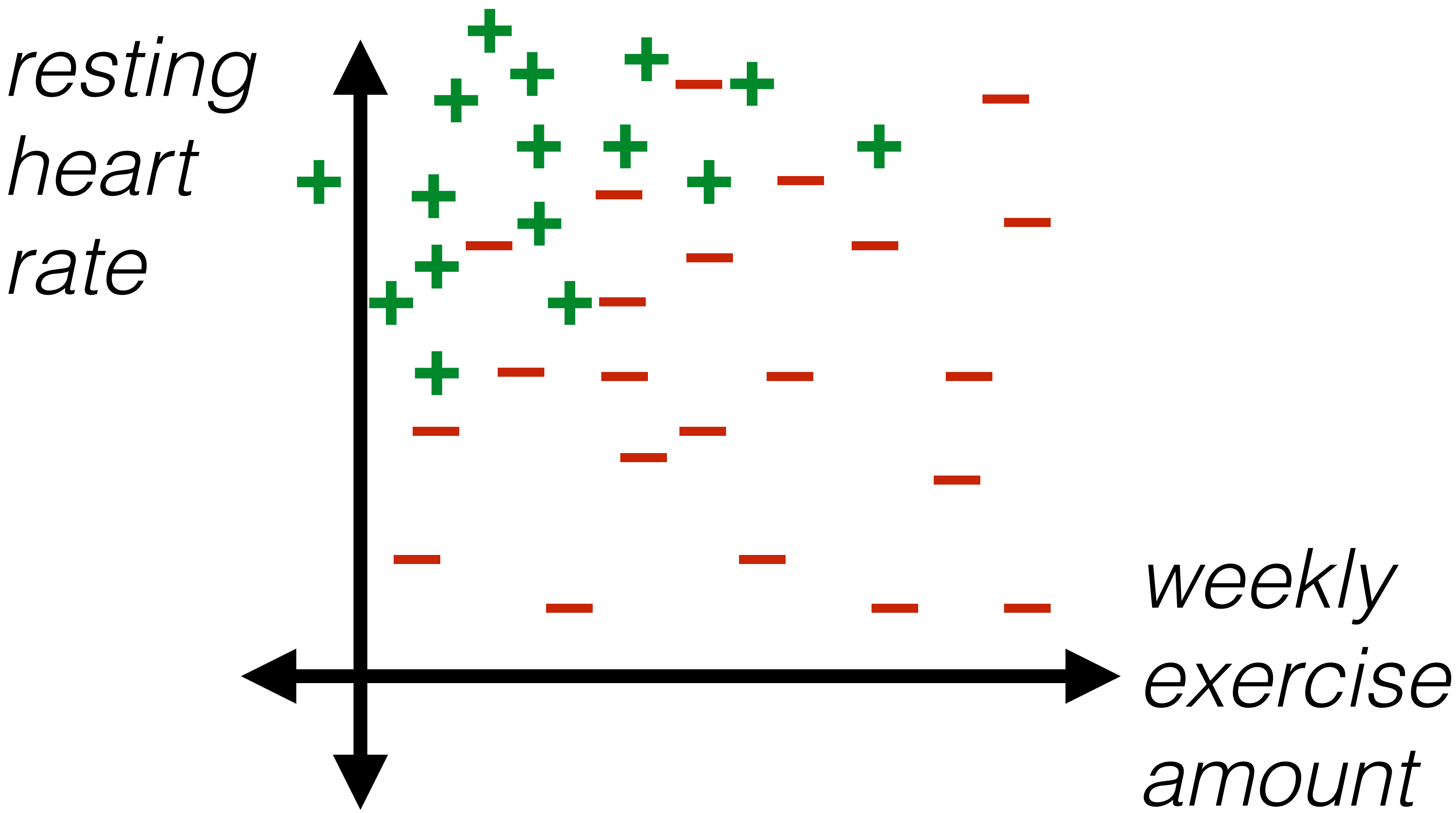

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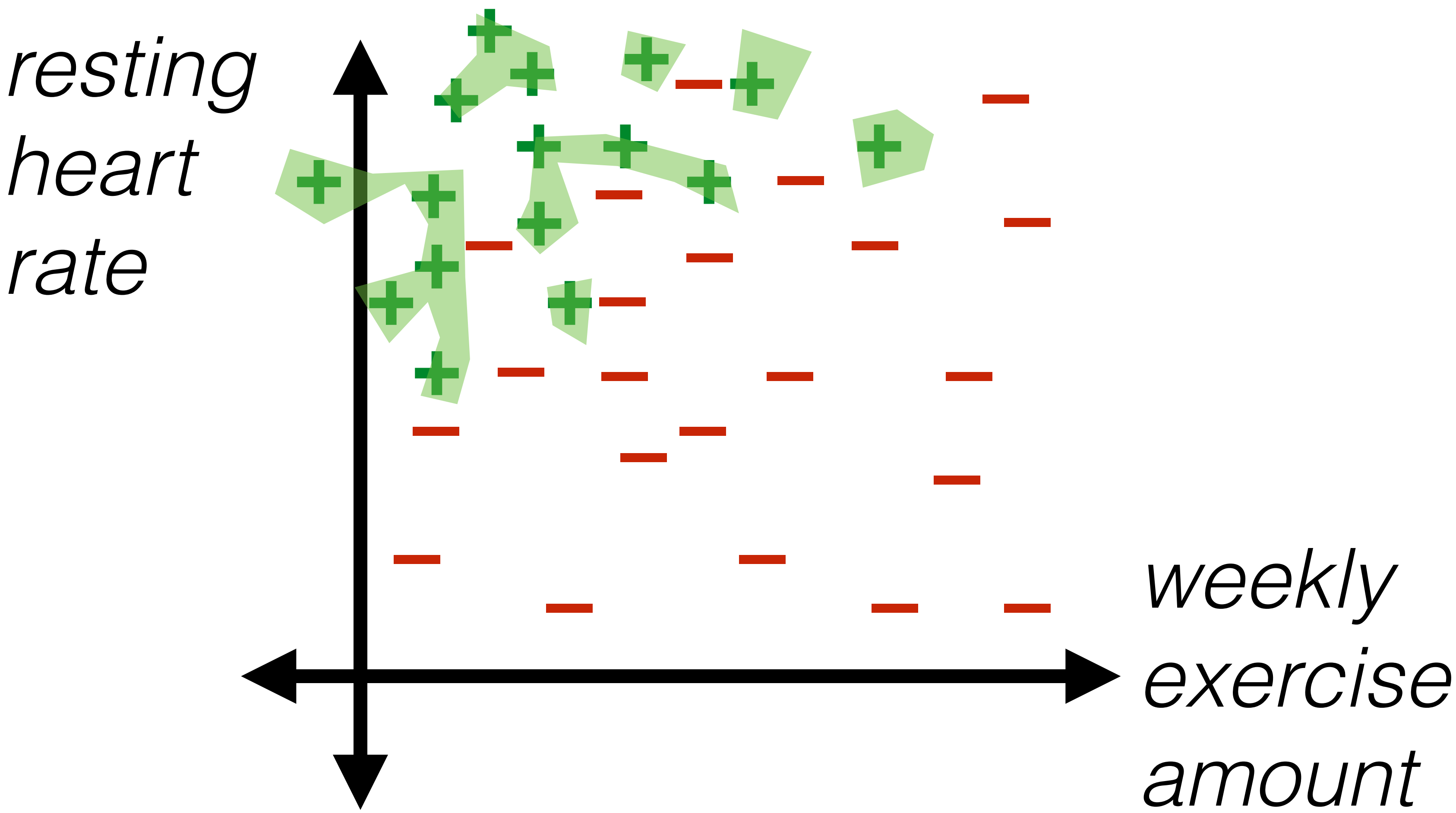

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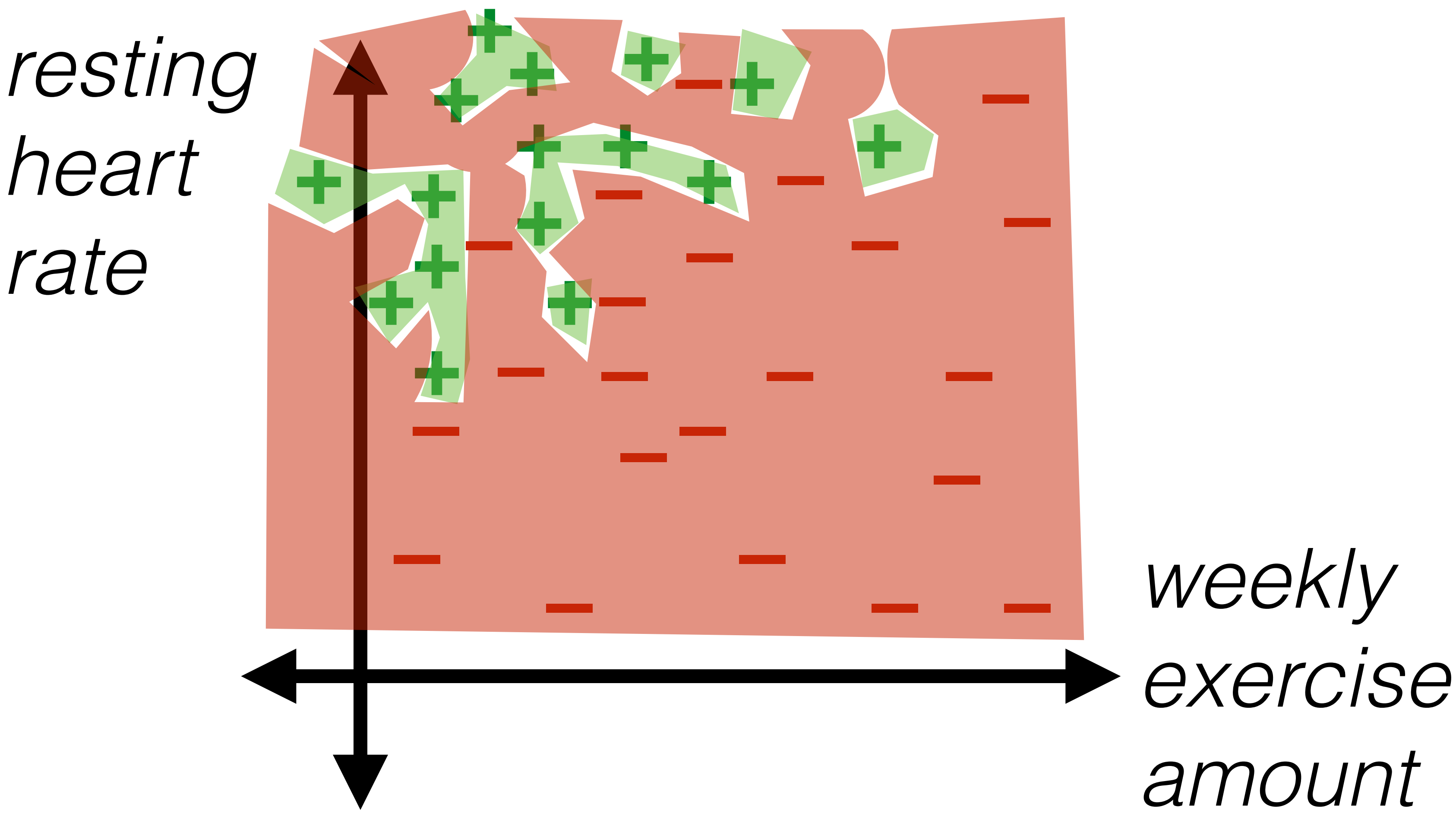
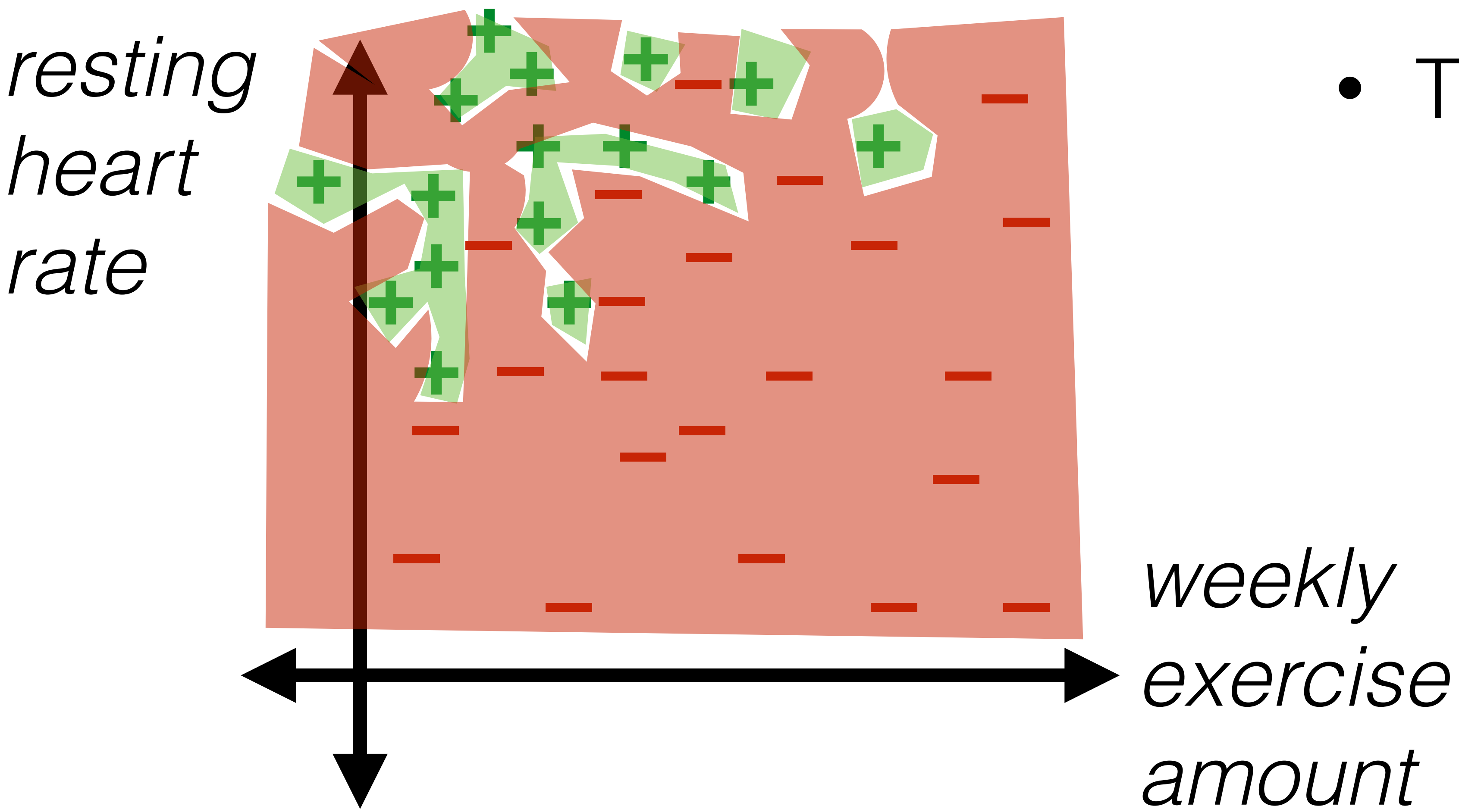
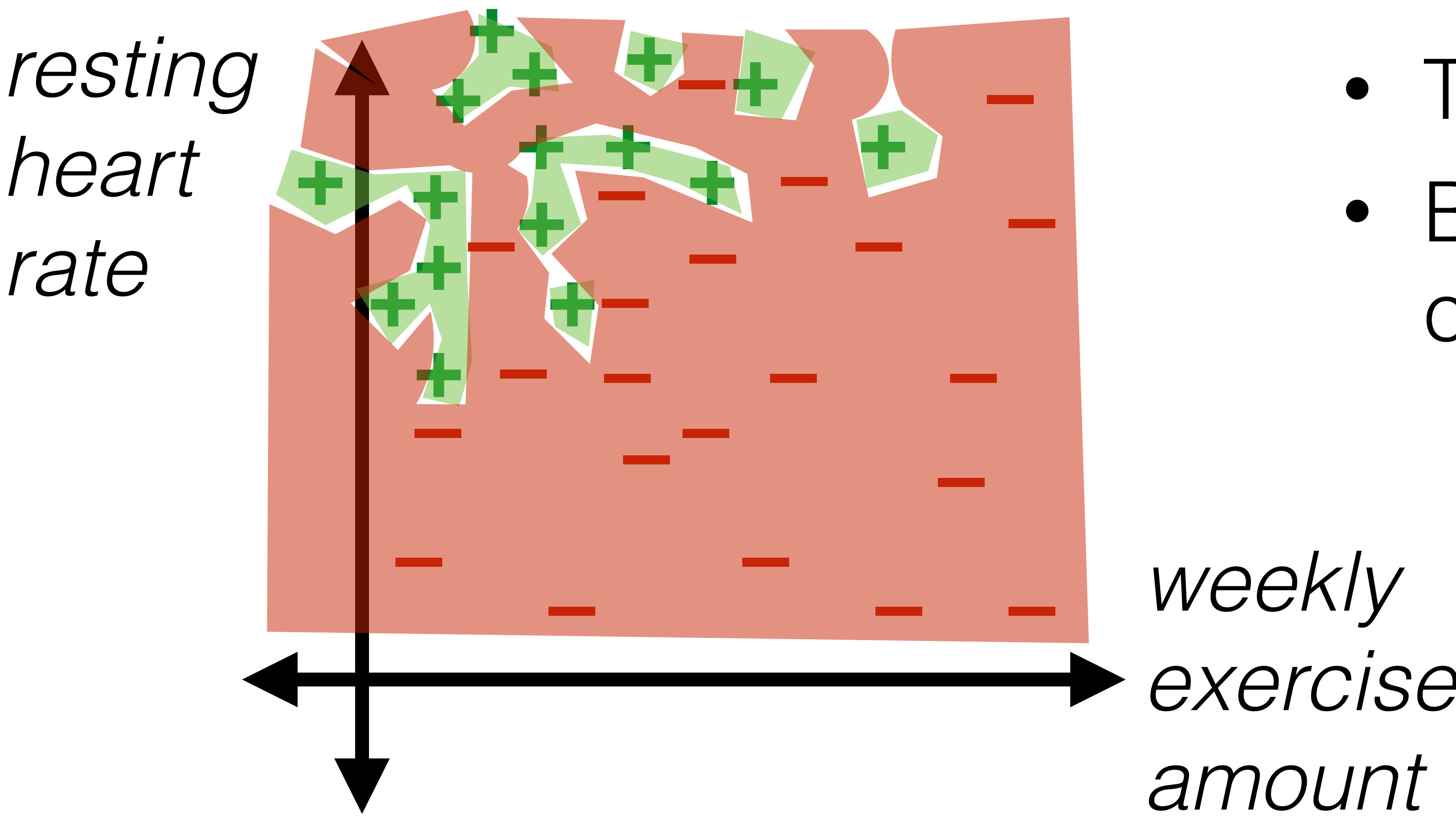


Nonlinear boundaries



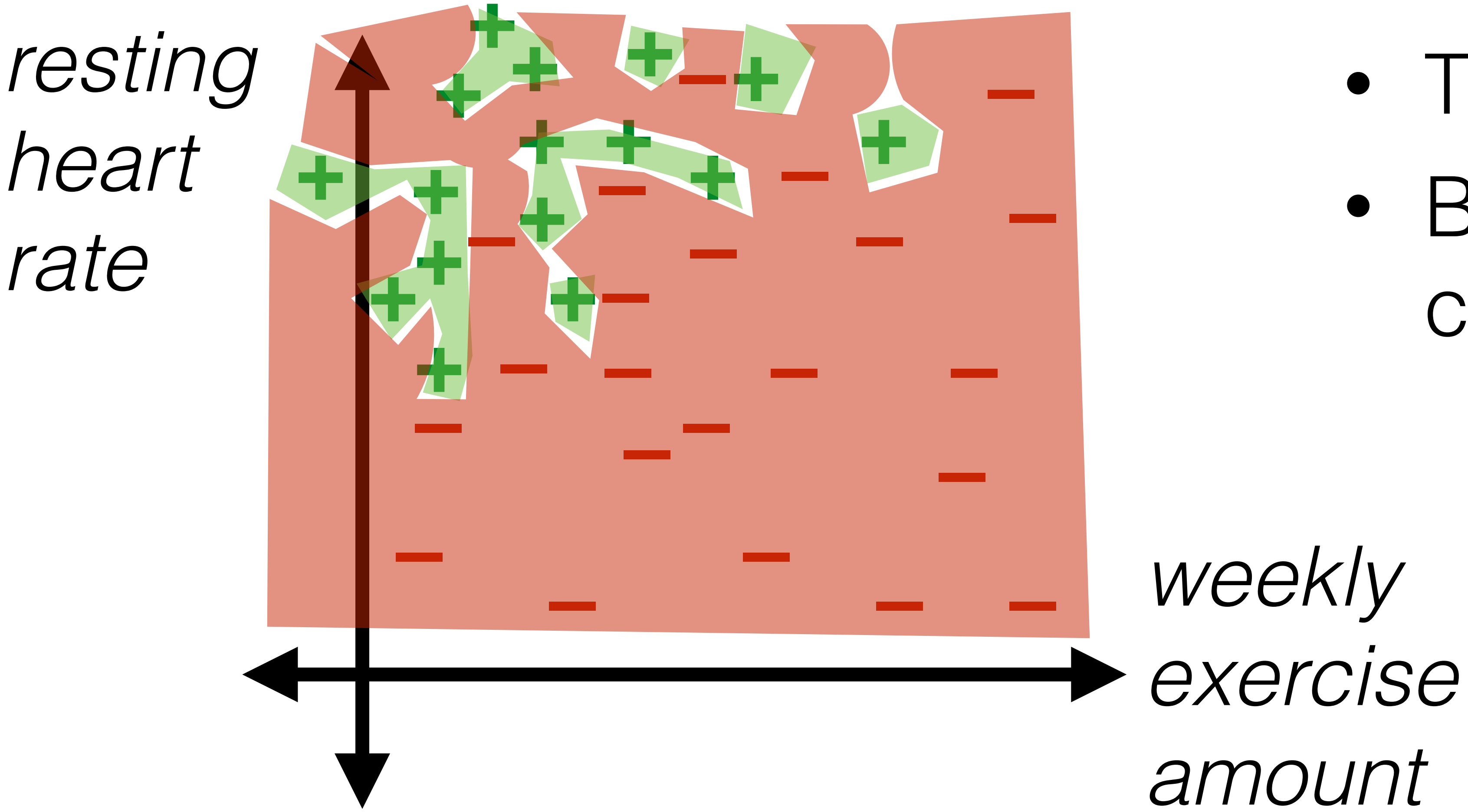
- Training error is 0!

Nonlinear boundaries



- Training error is 0!
- But seems like our classifier is overfitting

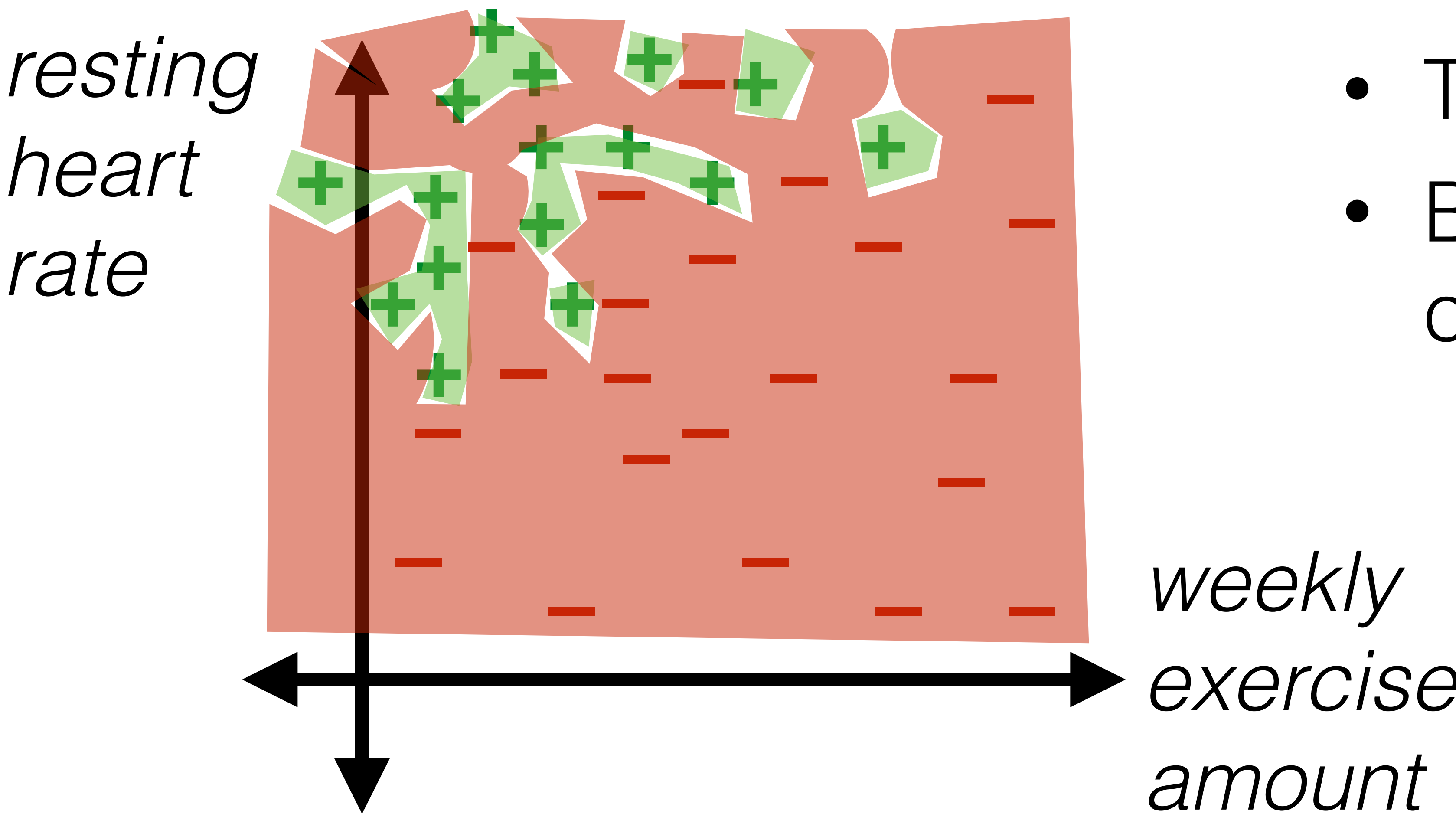
Nonlinear boundaries



- Training error is 0!
- But seems like our classifier is overfitting

- How can we detect overfitting?

Nonlinear boundaries



- Training error is 0!
- But seems like our classifier is overfitting

- How can we detect overfitting?
- How can we avoid overfitting?

Evaluation of a learning algorithm

- How good is our learning algorithm on data like ours?

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- Idea: use full data for training and then report training error

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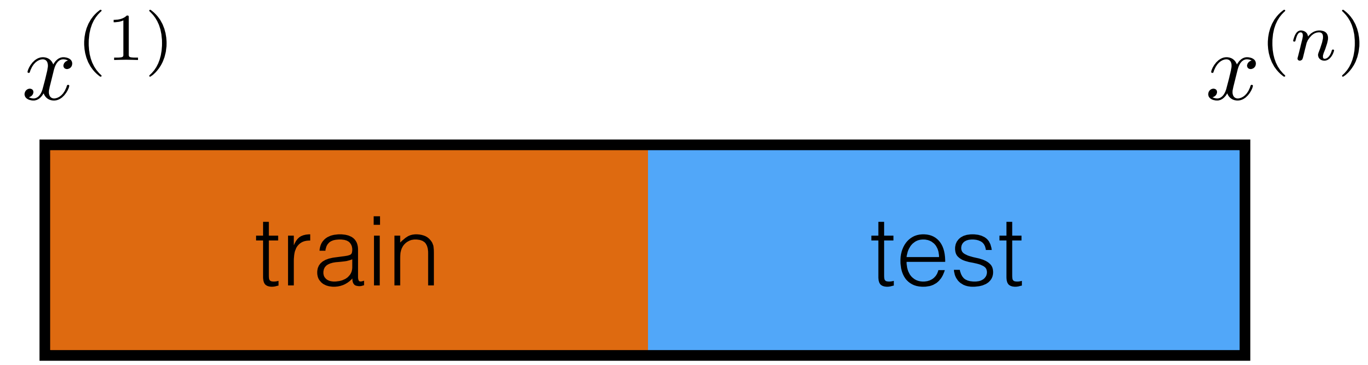

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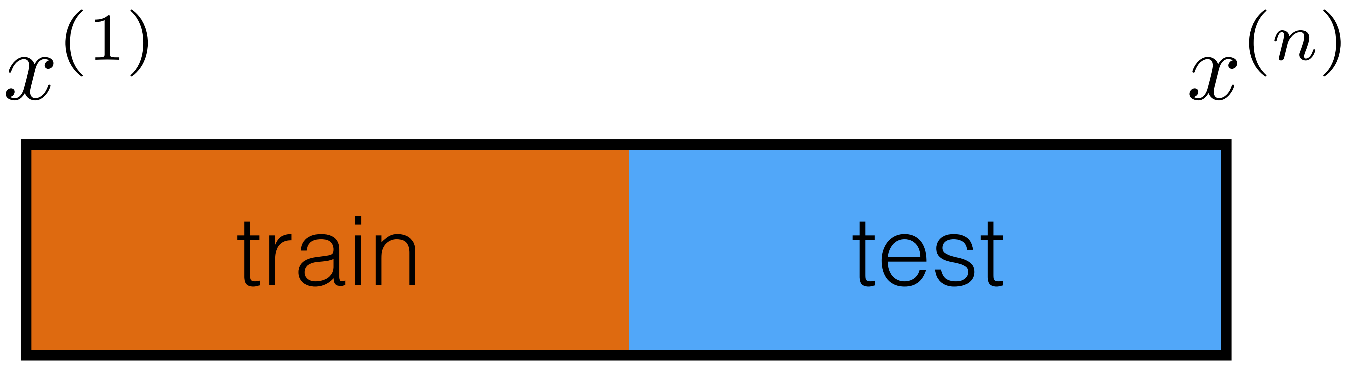
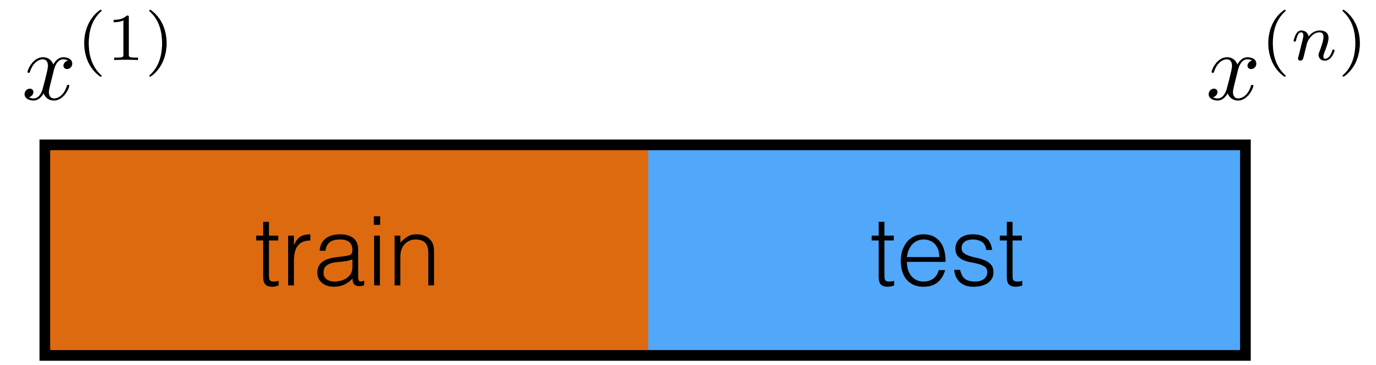


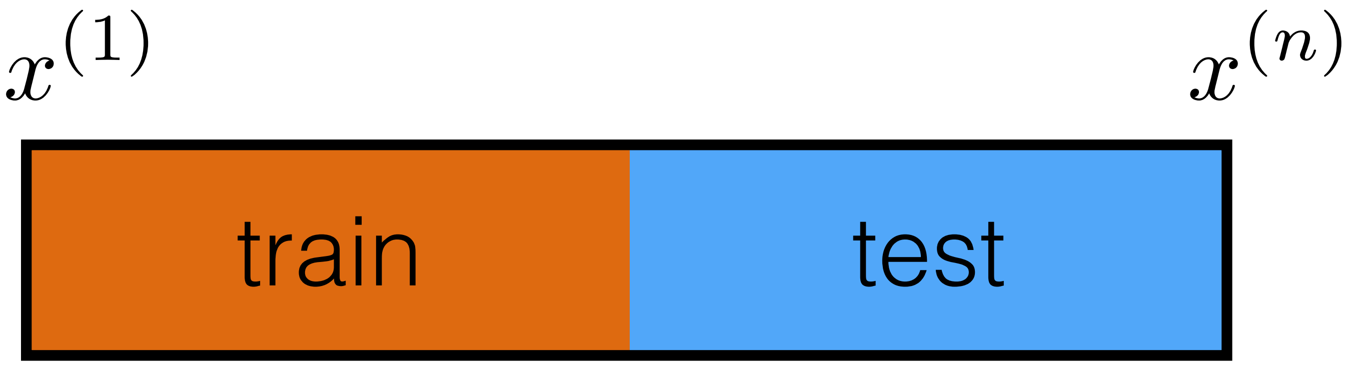
- How good is our learning algorithm on data like ours?
- Idea: use full data for training and then report training error
- Idea: reserve some data for testing
  - More training data: closer to training on full data

Evaluation of a learning algorithm



- How good is our learning algorithm on data like ours?
- Idea: use full data for training and then report training error
- Idea: reserve some data for testing
  - More training data: closer to training on full data
  - More testing data: less noisy estimate of performance

Evaluation of a learning algorithm



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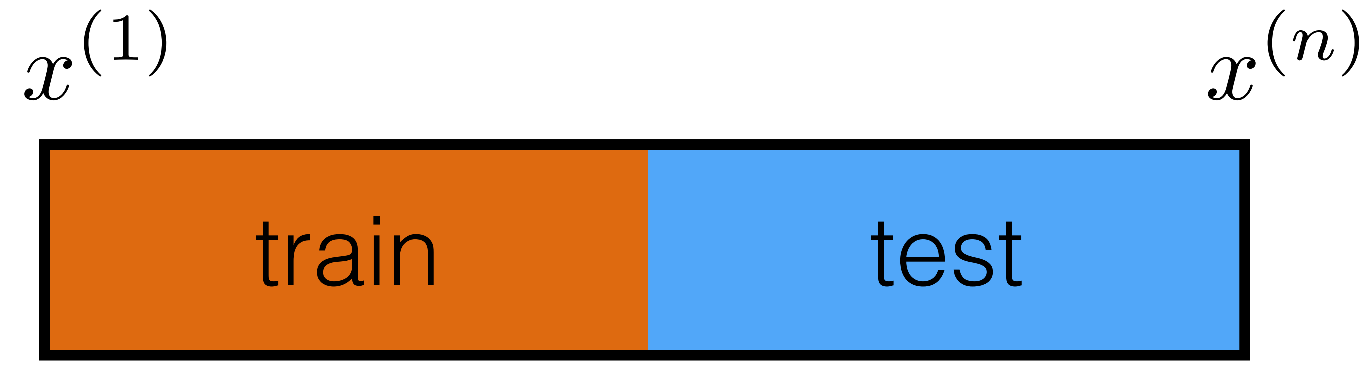
  - Only one classifier might not be representative

Evaluation of a learning algorithm



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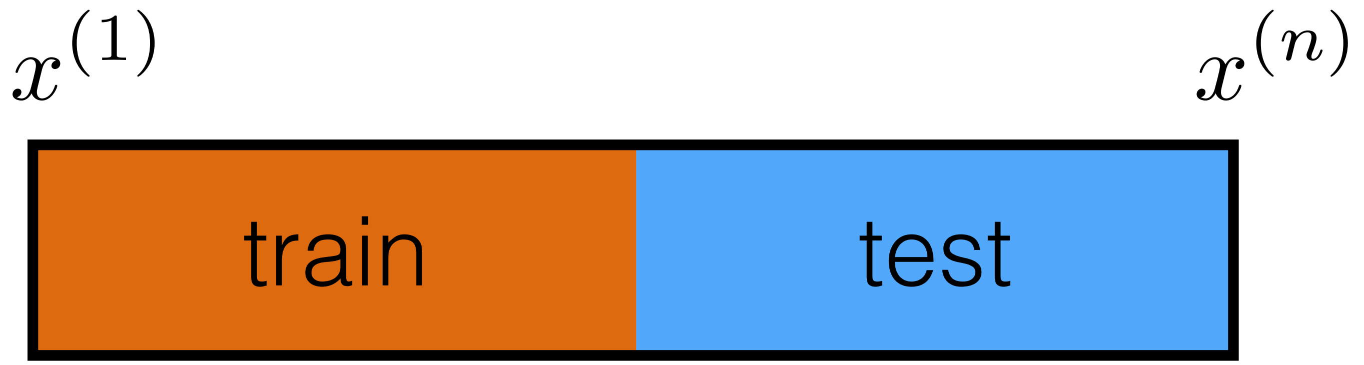

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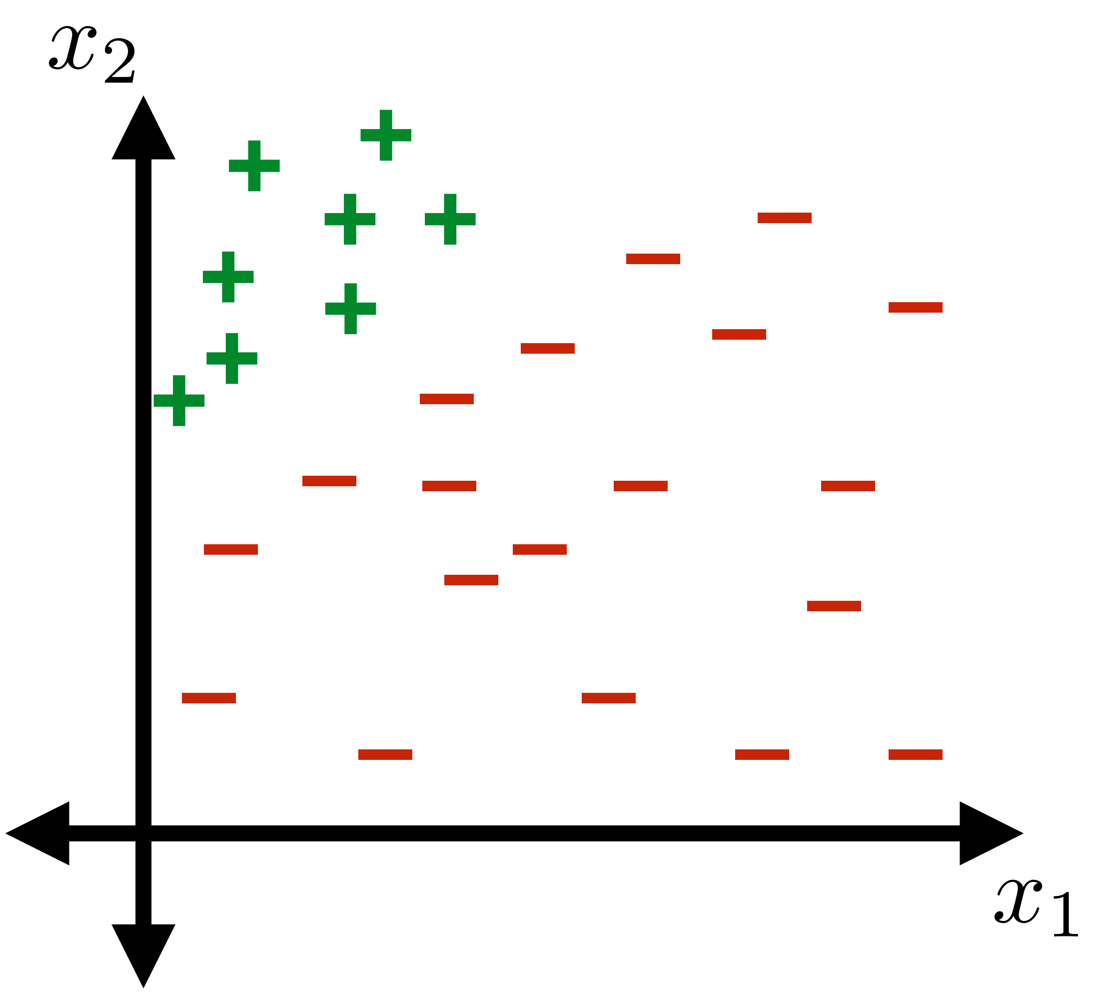

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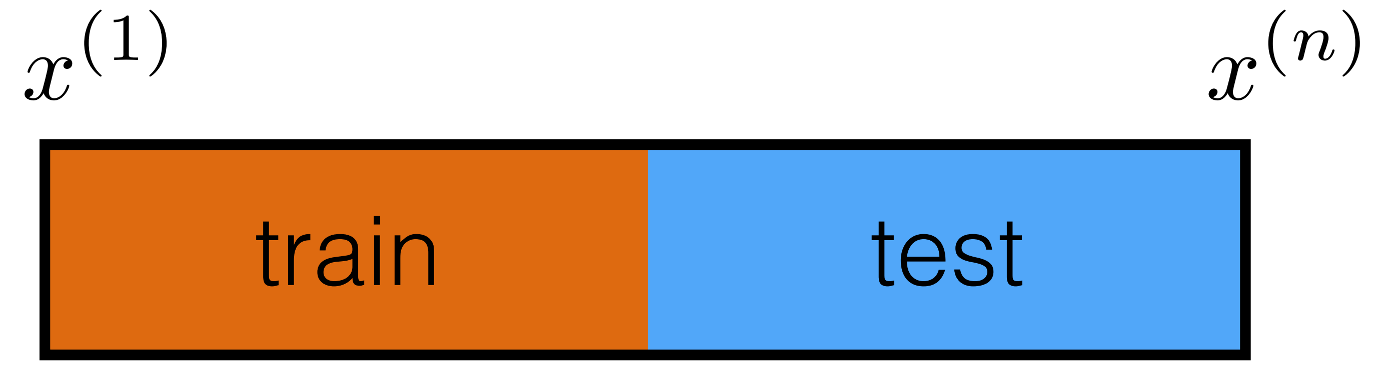

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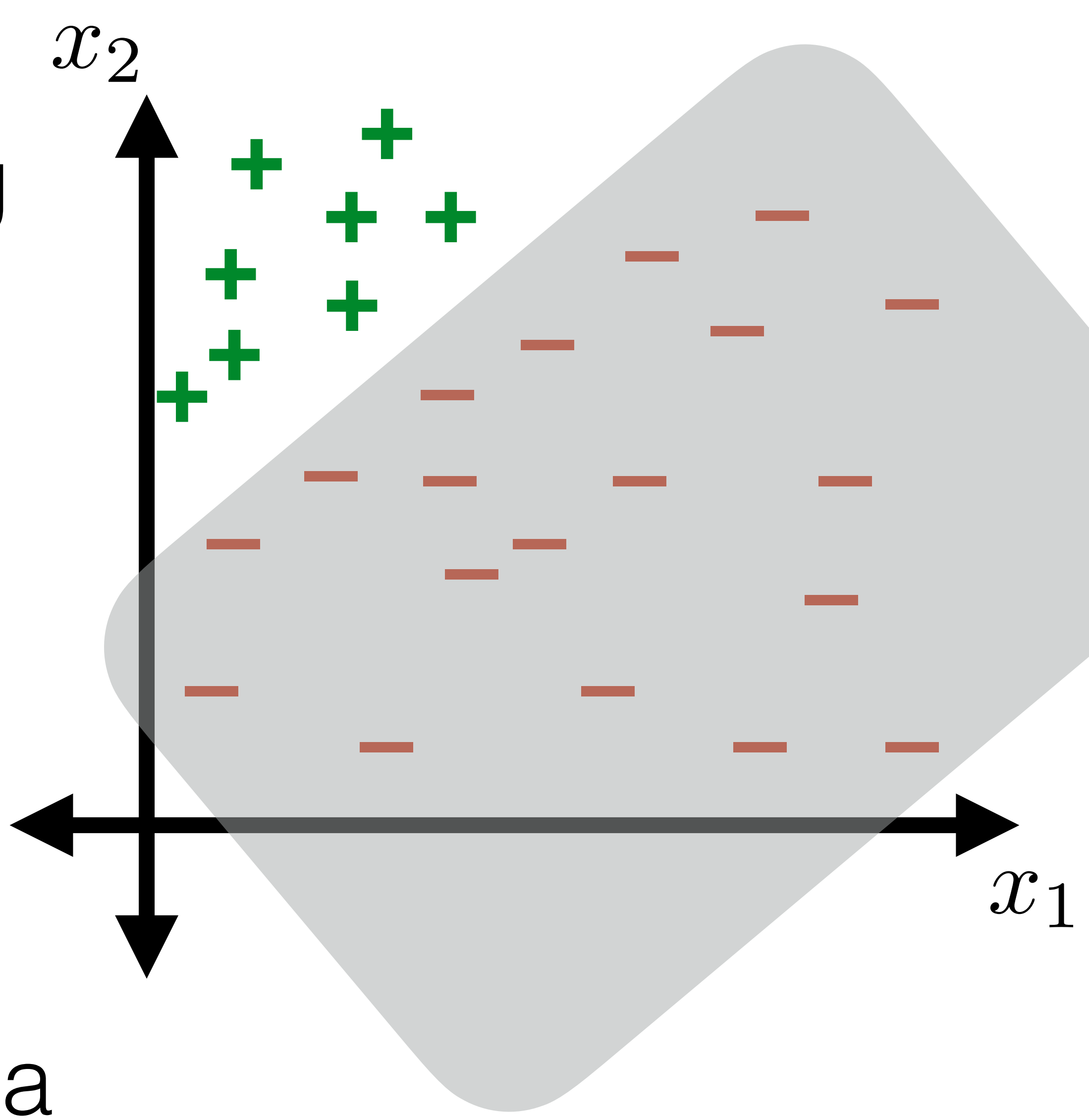

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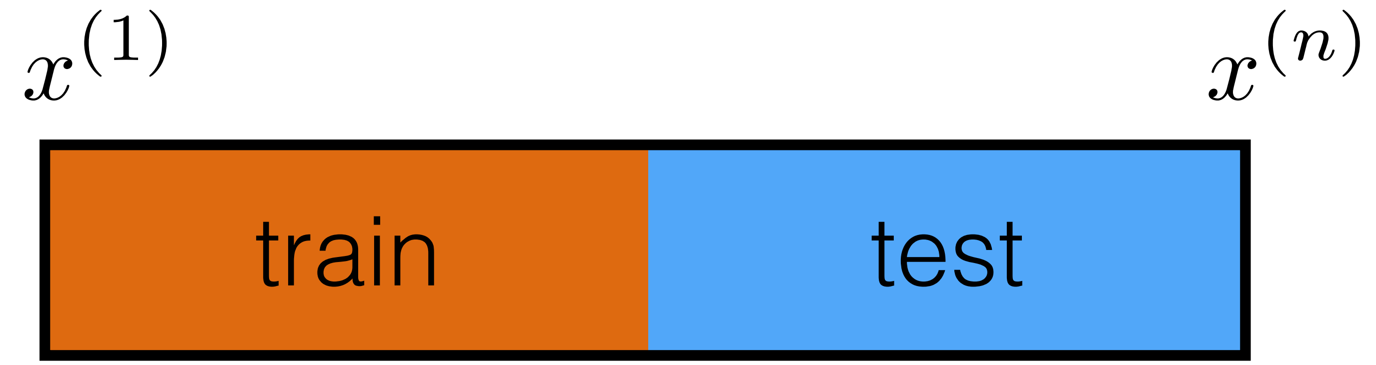

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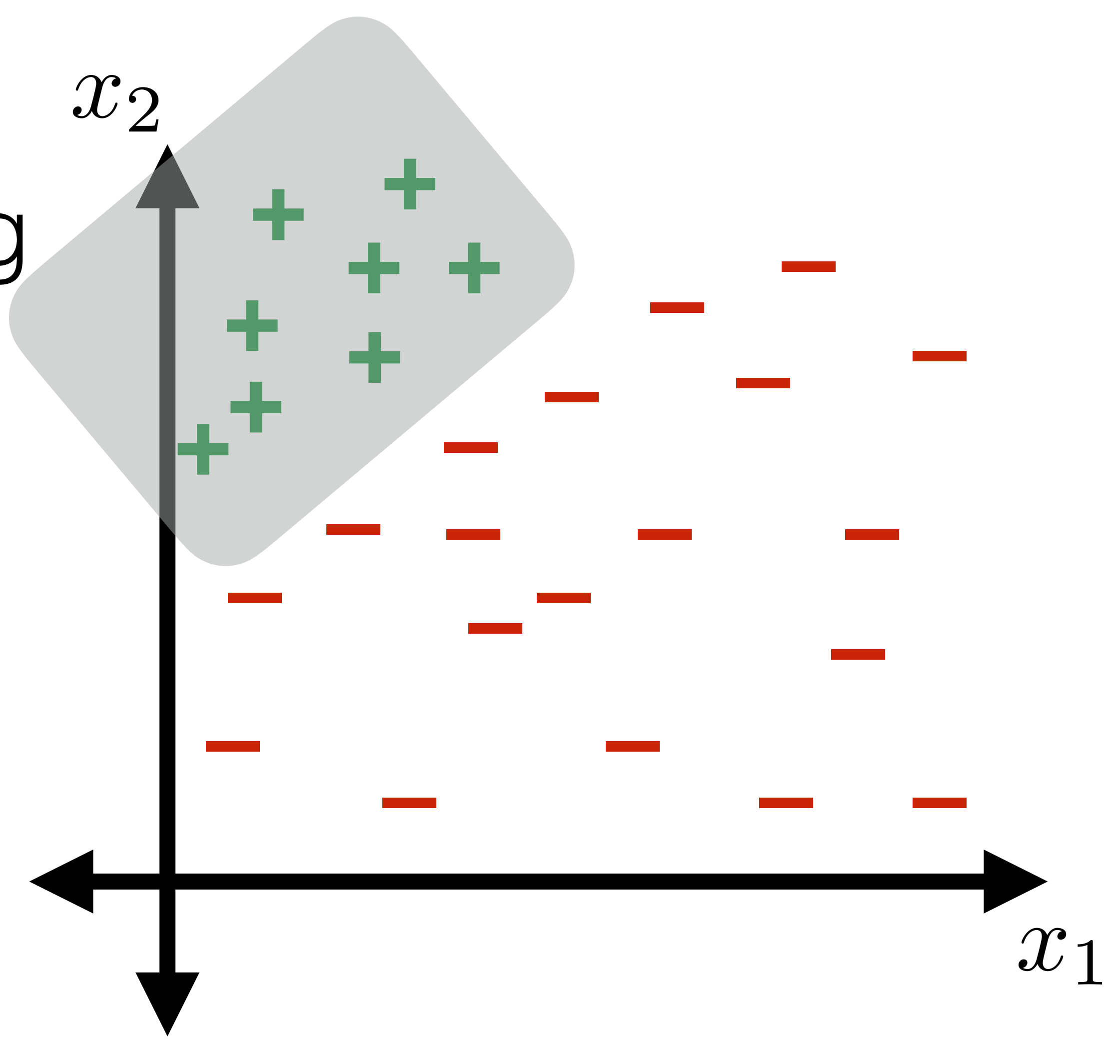


Evaluation of a learning algorithm

`Cross-validate(`$\mathcal{D}_n$ `,` k `)`

Evaluation of a learning algorithm

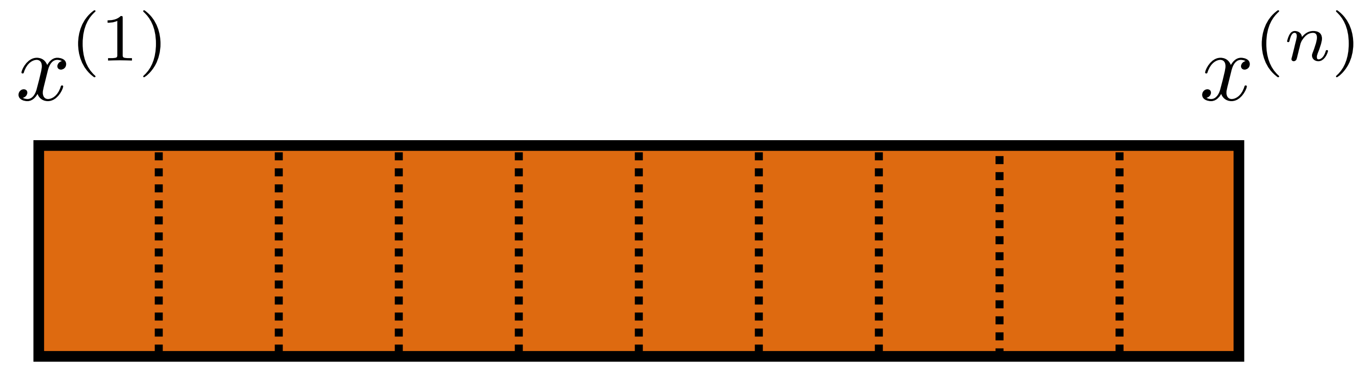
```
Cross-validate(D_n , k )
  Divide D_n into k chunks D_{n,1},...,D_{n,k} (of
  roughly equal size)
```

Evaluation of a learning algorithm

Cross-validate($\mathcal{D}_n$, k)

Divide $\mathcal{D}_n$ into k chunks $\mathcal{D}_{n,1}, \ldots, \mathcal{D}_{n,k}$ (of roughly equal size)

Evaluation of a learning algorithm



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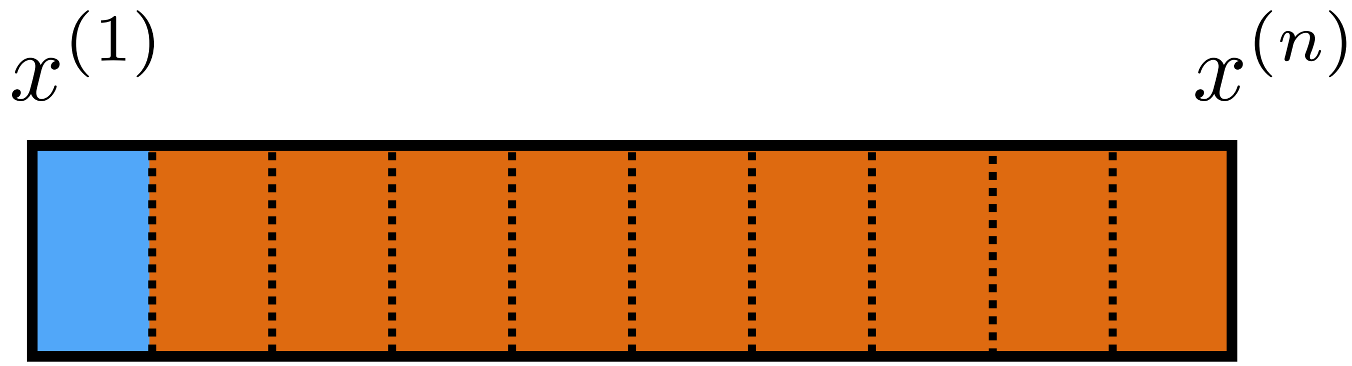
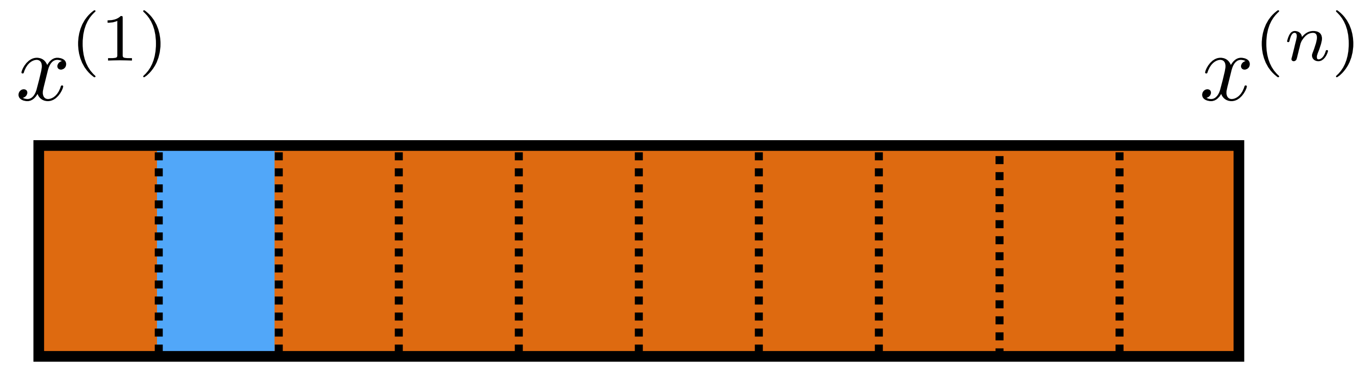
Divide $\mathcal{D}_n$ into k chunks $\mathcal{D}_{n,1}, \ldots, \mathcal{D}_{n,k}$ (of roughly equal size)

Evaluation of a learning algorithm




```
Cross-validate( $\mathcal{D}_n$ , $k$ )
  Divide $\mathcal{D}_n$ into $k$ chunks $\mathcal{D}_{n,1},\ldots,\mathcal{D}_{n,k}$ (of
  roughly equal size)
  for i = 1 to $k$
```

Evaluation of a learning algorithm

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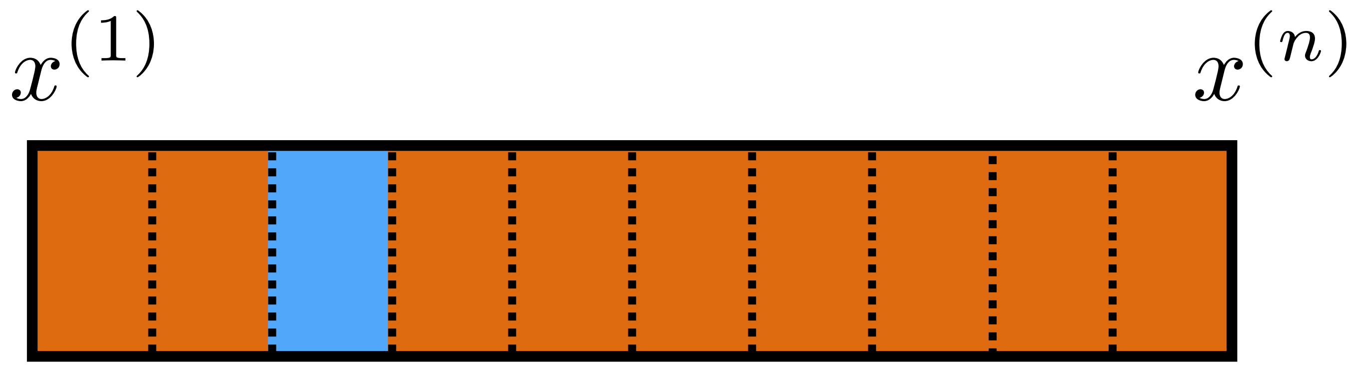

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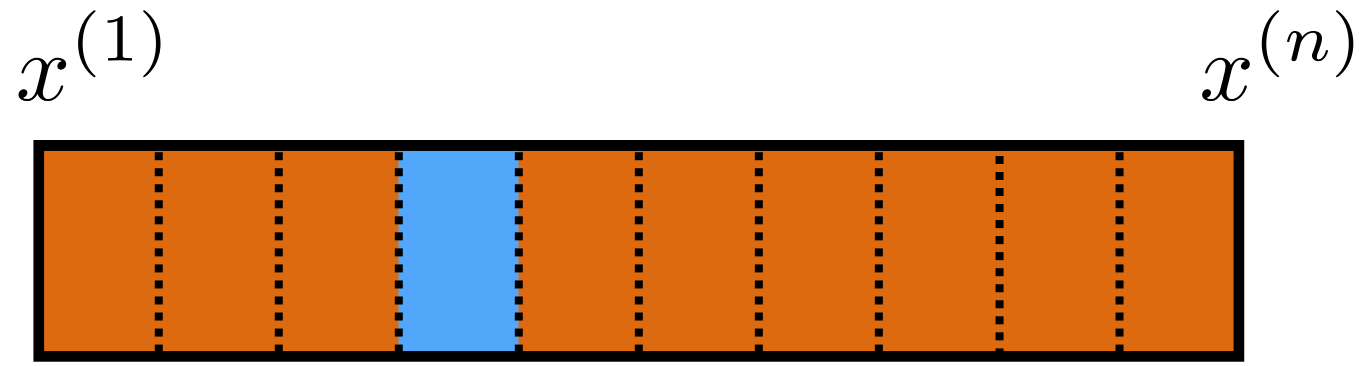


```
Cross-validate( 𝒟_n , k )
  Divide 𝒟_n into k chunks 𝒟_{n,1}, ..., 𝒟_{n,k} (of
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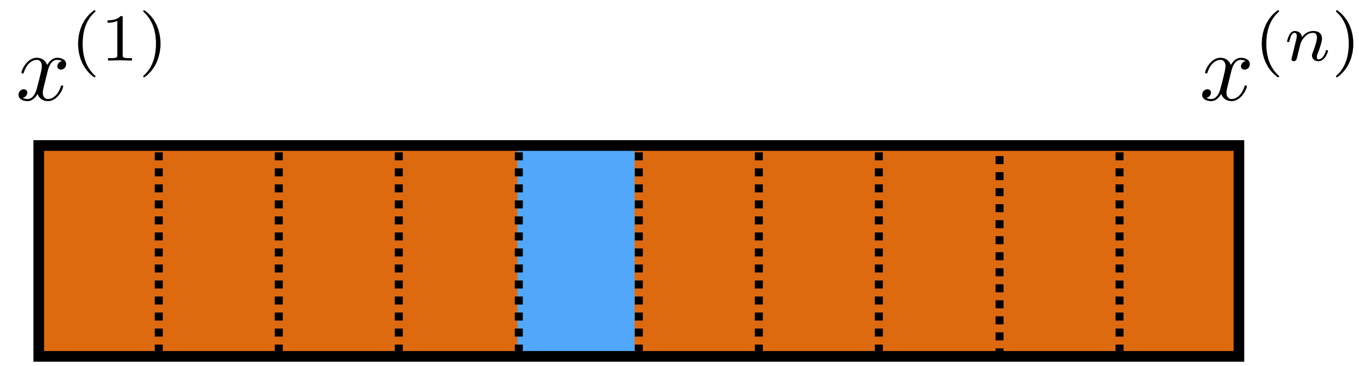


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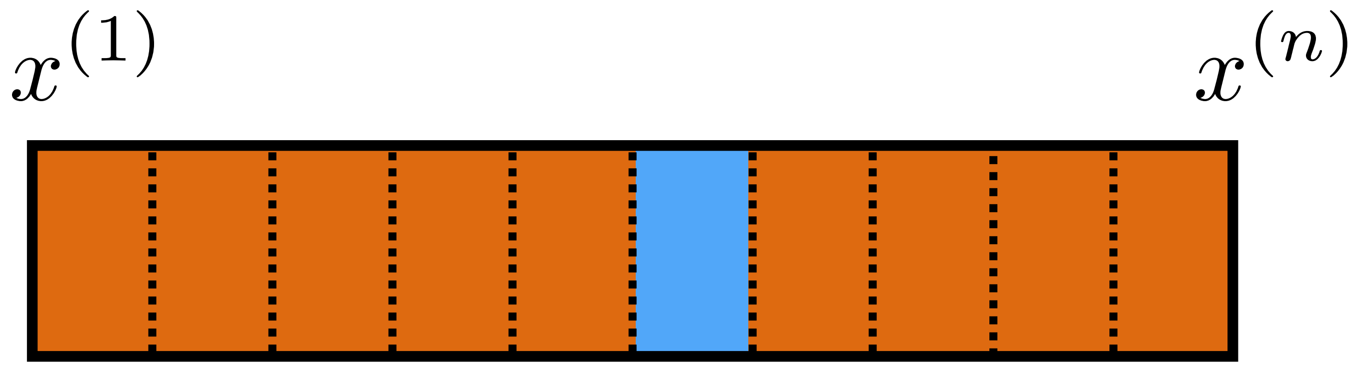

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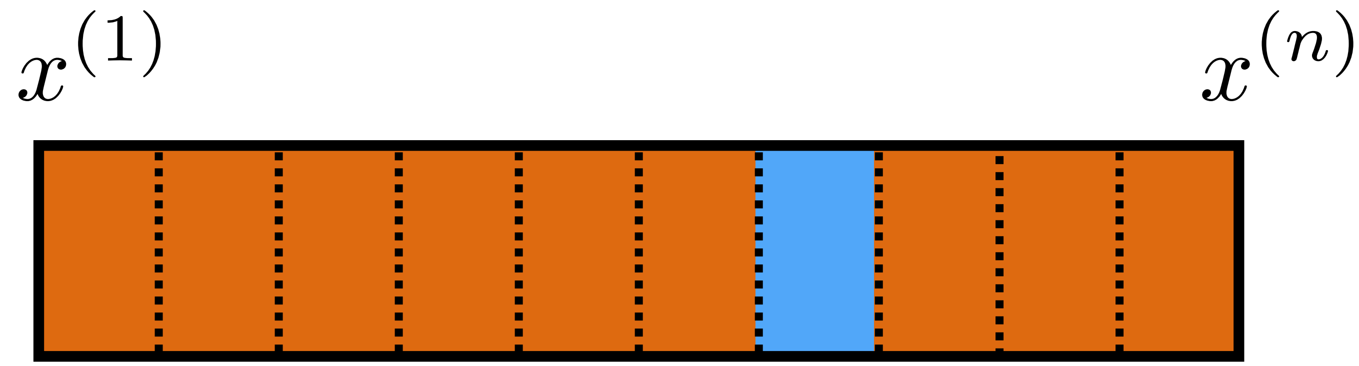


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Cross-validate( $\mathcal{D}_n$ , $k$ )
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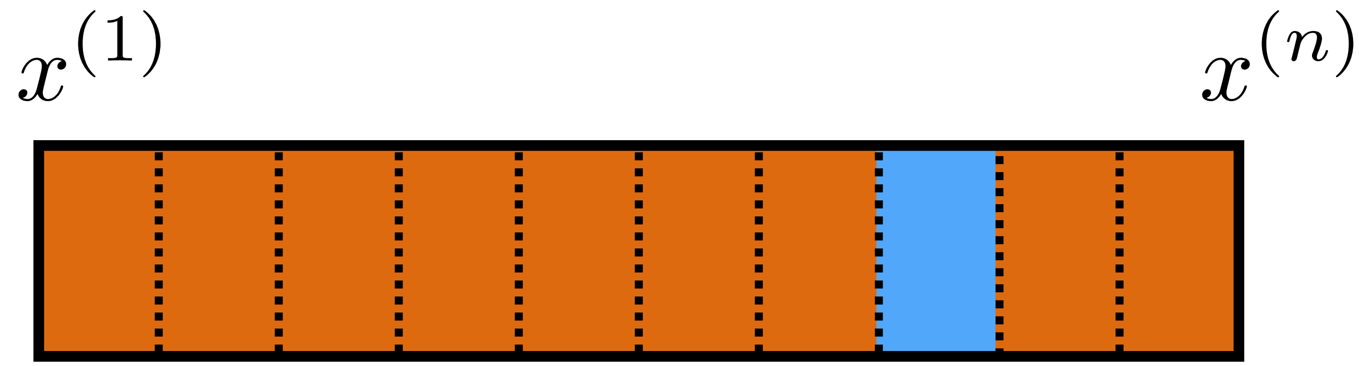

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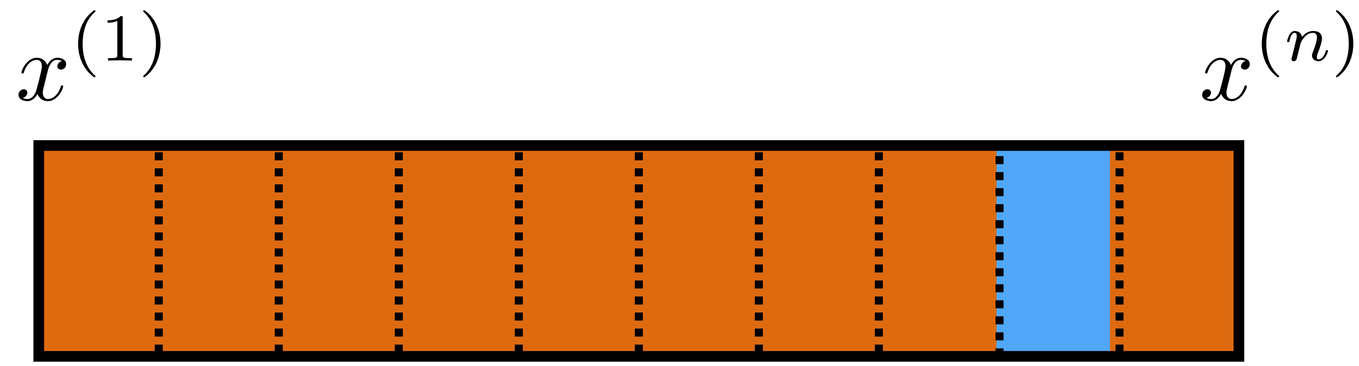


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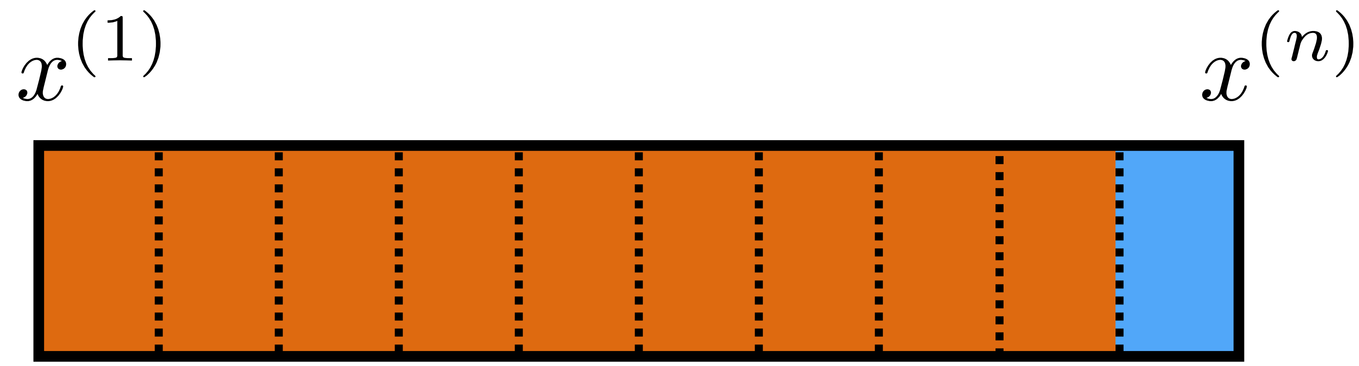
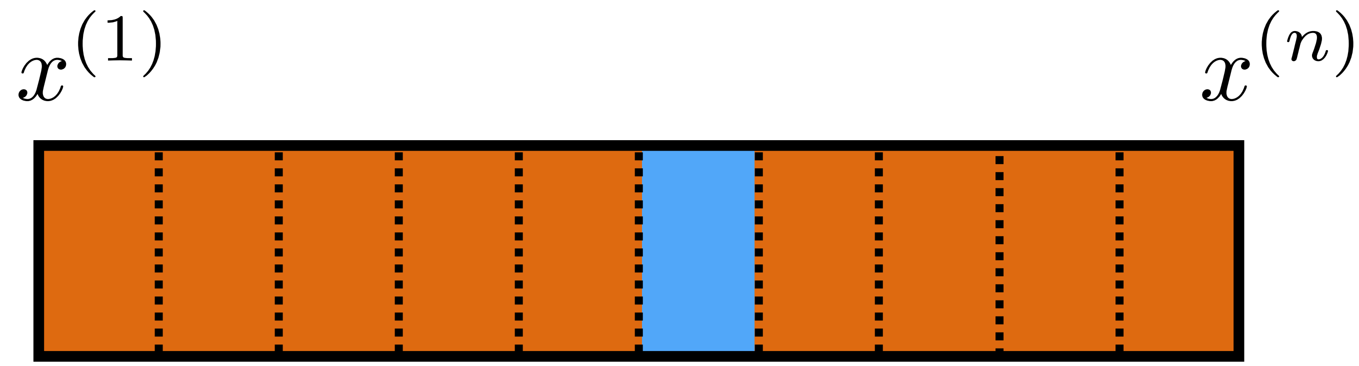
Evaluation of a learning algorithm



```
Cross-validate( 𝒟ₙ , k )
  Divide 𝒟ₙ into k chunks 𝒟ₙ,₁,...,𝒟ₙ,ₖ (of
  roughly equal size)
  for i = 1 to k
```

Evaluation of a learning algorithm




```
Cross-validate( 𝒟_n , k )
  Divide 𝒟_n into k chunks 𝒟_{n,1}, ..., 𝒟_{n,k} (of
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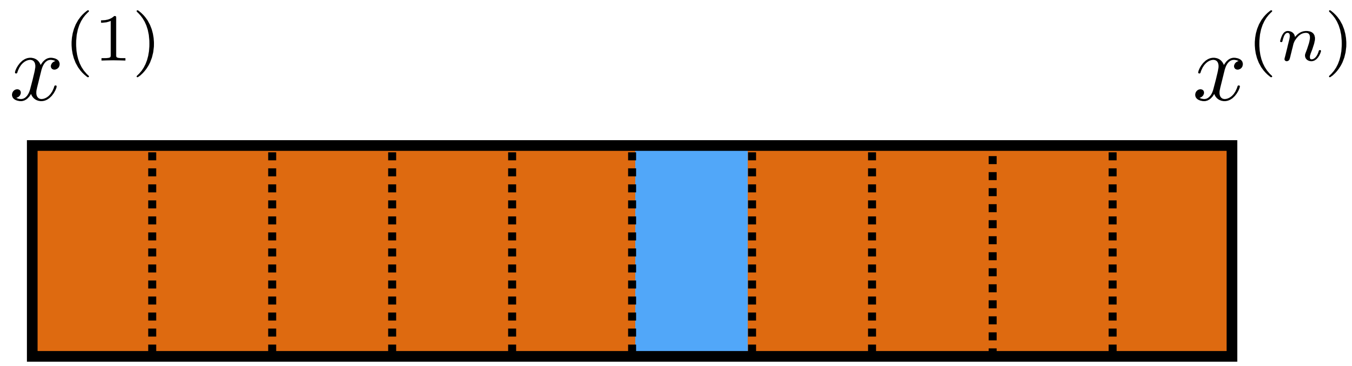
```

Cross-validate($\mathcal{D}_n$, k)

Divide $\mathcal{D}_n$ into k chunks $\mathcal{D}_{n,1}, \ldots, \mathcal{D}_{n,k}$ (of roughly equal size)

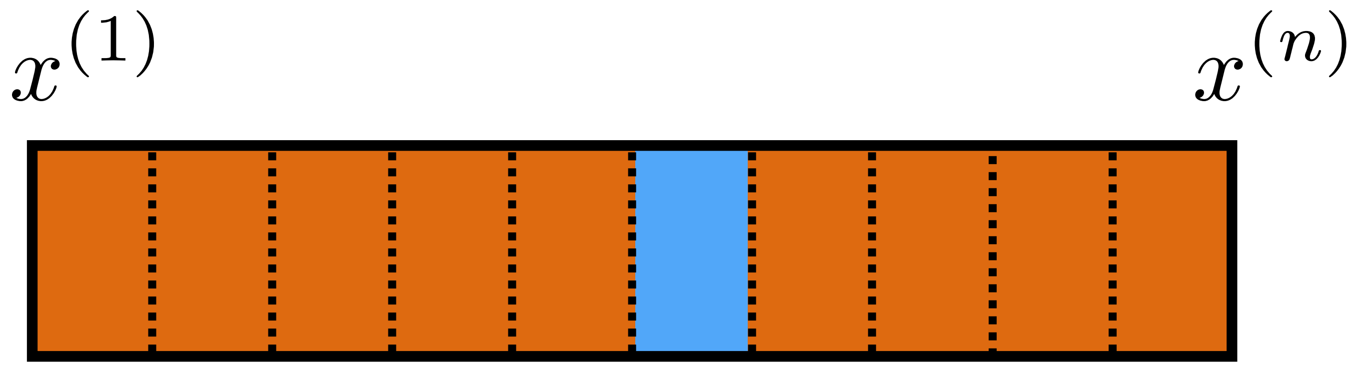
for i = 1 to k

Evaluation of a learning algorithm



```
Cross-validate( $\mathcal{D}_n$ , $k$ )
  Divide $\mathcal{D}_n$ into $k$ chunks $\mathcal{D}_{n,1},\ldots,\mathcal{D}_{n,k}$ (of
  roughly equal size)
  for i = 1 to $k$
    train $h_i$ on $\mathcal{D}_n \backslash \mathcal{D}_{n,i}$ (i.e. except chunk i)
```

Evaluation of a learning algorithm



Cross-validate($\mathcal{D}_n$, k)

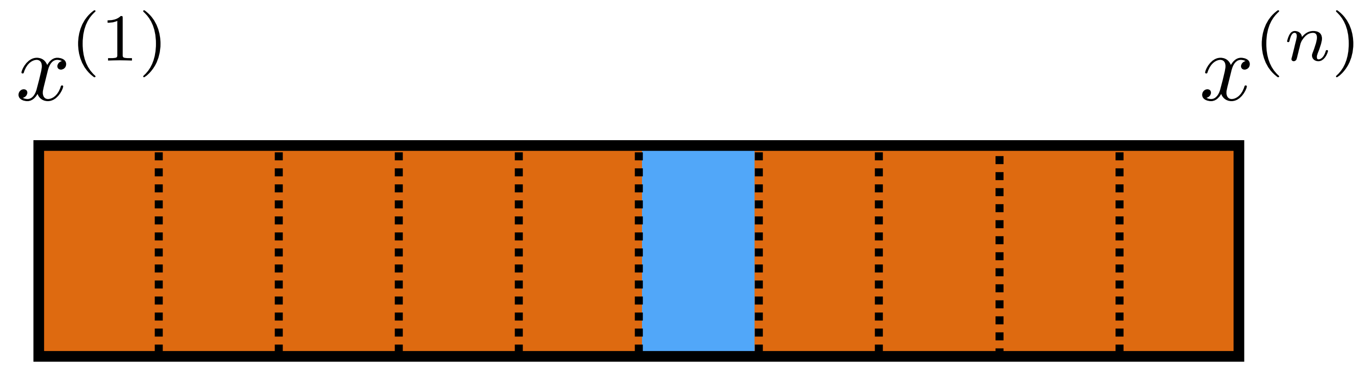
  Divide $\mathcal{D}_n$ into k chunks $\mathcal{D}_{n,1}, \ldots, \mathcal{D}_{n,k}$ (of roughly equal size)

  for i = 1 to k

    train h_i on $\mathcal{D}_n \backslash \mathcal{D}_{n,i}$ (i.e. except chunk i)

    compute "test" error $\mathcal{E}(h_i, \mathcal{D}_{n,i})$ of h_i on $\mathcal{D}_{n,i}$

Evaluation of a learning algorithm



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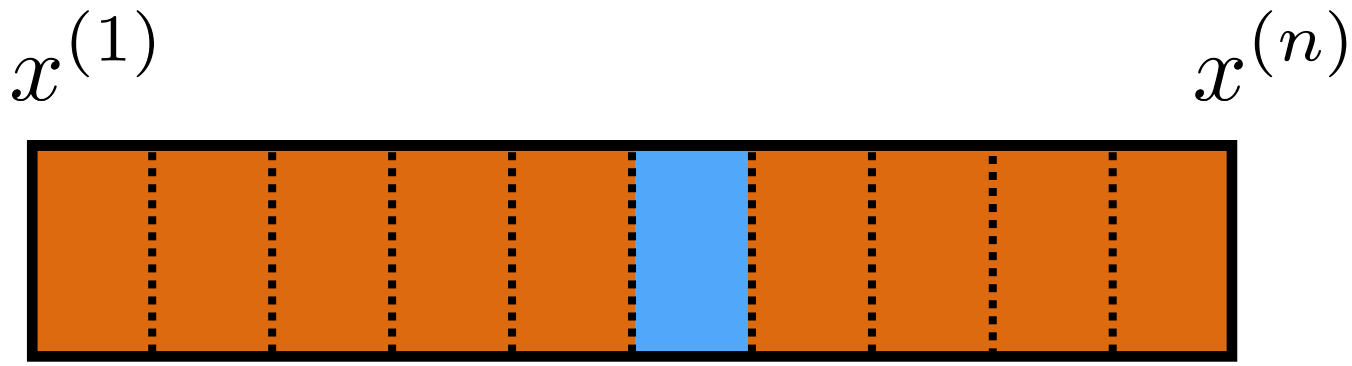
    compute "test" error $\mathcal{E}(h_i, \mathcal{D}_{n,i})$ of h_i on $\mathcal{D}_{n,i}$

  Return $\frac{1}{k}\sum_{i=1}^{k} \mathcal{E}(h_i, \mathcal{D}_{n,i})$

Evaluation of a learning algorithm



```
Cross-validate( 𝒟ₙ , k )
  Divide 𝒟ₙ into k chunks 𝒟ₙ,₁,...,𝒟ₙ,ₖ (of
  roughly equal size)
  for i = 1 to k
    train hᵢ on 𝒟ₙ\𝒟ₙ,ᵢ (i.e. except chunk i)
    compute "test" error ℰ(hᵢ,𝒟ₙ,ᵢ) of hᵢ on 𝒟ₙ,ᵢ
  Return (1/k) Σᵢ₌₁ᵏ ℰ(hᵢ,𝒟ₙ,ᵢ)
```

Cross-validate($\mathcal{D}_n$, k)

Divide $\mathcal{D}_n$ into k chunks $\mathcal{D}_{n,1},\ldots,\mathcal{D}_{n,k}$ (of roughly equal size)

for i = 1 to k

train h_i on $\mathcal{D}_n \backslash \mathcal{D}_{n,i}$ (i.e. except chunk i)

compute "test" error $\mathcal{E}(h_i, \mathcal{D}_{n,i})$ of h_i on $\mathcal{D}_{n,i}$

Return $\frac{1}{k}\sum_{i=1}^{k}\mathcal{E}(h_i, \mathcal{D}_{n,i})$

- Again, good idea to shuffle order of data first