MinNorm approximation of MaxEnt/MinDiv problems for probability tables

Patrick Bogaert and Sarah Gengler
Rebuilding probability tables
Rebuilding probability tables

• Limited number of samples → Poor estimates
Rebuilding probability tables

• Limited number of samples ⇐ Poor estimates

• How to integrate experts opinion?
Rebuilding probability tables

• Limited number of samples \implies Poor estimates

• How to integrate experts opinion?

\implies Rewriting information as \textit{equality} / \textit{inequality} constraints
Rebuilding probability tables

• Limited number of samples $\Rightarrow$ Poor estimates

• How to integrate experts opinion?

$\Rightarrow$ Rewriting information as **equality** / **inequality** constraints
Rebuilding probability tables

• Limited number of samples ⇒ Poor estimates

• How to integrate experts opinion?

⇒ Rewriting information as equality / inequality constraints

• Equality constraints ⇒ MaxEnt
  • Inequality constraints ⇒ Minimum divergence (MinDiv)
Rebuilding probability tables

• Limited number of samples $\Rightarrow$ Poor estimates

• How to integrate experts opinion?

$\Rightarrow$ Rewriting information as equality / inequality constraints

• Equality constraints $\Rightarrow$ MaxEnt

• Inequality constraints $\Rightarrow$ Minimum divergence (MinDiv)

$\Rightarrow$ Need for an efficient methodology to rebuild probability tables from both equality and inequality constraints
The MaxEnt problem
The MaxEnt problem

• Equality constraints

\[
\begin{cases}
    a'_1 p = b_1 \\
    \vdots \\
    a'_k p = b_k \\
    1' p = 1
\end{cases}
\iff
\begin{pmatrix}
    a_{11} & \cdots & a_{1n} \\
    \vdots & \ddots & \vdots \\
    a_{k1} & \cdots & a_{kn}
\end{pmatrix}
\begin{pmatrix}
    p_1 \\
    \vdots \\
    p_n
\end{pmatrix}
= 
\begin{pmatrix}
    b_1 \\
    \vdots \\
    b_k
\end{pmatrix}
\iff
A p = b
\]
The MaxEnt problem

• Equality constraints

\[
\begin{cases}
    a_1' p = b_1 \\
    \vdots \\
    a_k' p = b_k \\
    1' p = 1
\end{cases}
\iff
\begin{pmatrix}
    a_{11} & \cdots & a_{1n} \\
    \vdots & \ddots & \vdots \\
    a_{k1} & \cdots & a_{kn}
\end{pmatrix} \begin{pmatrix}
    p_1 \\
    \vdots \\
    p_n
\end{pmatrix} = \begin{pmatrix}
    b_1 \\
    \vdots \\
    b_k
\end{pmatrix}
\iff
Ap = b
\]

• Entropy maximized subject to the equality constraints

\[
O(p, \mu) = H(p) + \mu' (Ap - b)
\]

\[
\begin{cases}
    \frac{\partial O(p, \mu)}{\partial p} = -\ln p - 1 + A' \mu = 0 \\
    \frac{\partial O(p, \mu)}{\partial \mu} = Ap - b = 0
\end{cases}
\]
The MaxEnt problem

• Equality constraints

\[
\begin{align*}
\begin{cases}
 a'_1 p = b_1 \\
 \vdots \\
 a'_k p = b_k \\
 1' p = 1
\end{cases}
\end{align*}
\]  \iff  
\[
\begin{pmatrix}
 a_{11} & \cdots & a_{1n} \\
 \vdots & \ddots & \vdots \\
 a_{k1} & \cdots & a_{kn}
\end{pmatrix}
\begin{pmatrix}
 p \\
 \vdots \\
 1
\end{pmatrix} =
\begin{pmatrix}
 b_1 \\
 \vdots \\
 b_k
\end{pmatrix}
\iff
A p = b
\]

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O(p, \mu) = H(p) + \mu' (A p - b)
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\begin{align*}
\frac{\partial O(p, \mu)}{\partial p} &= -\ln p - 1 + A' \mu = 0 \\
\frac{\partial O(p, \mu)}{\partial \mu} &= A p - b = 0
\end{align*}
\]  \iff  
\[
\begin{pmatrix}
 0 & A' \\
 A & 0
\end{pmatrix}
\begin{pmatrix}
 p \\
 \mu
\end{pmatrix} =
\begin{pmatrix}
 \ln p + 1 \\
 b
\end{pmatrix}
\]
The MaxEnt problem

• Equality constraints

\[
\begin{align*}
\begin{cases}
a'_1 p = b_1 \\
\vdots \\
a'_k p = b_k \\
p' = 1
\end{cases}
\iff
\begin{pmatrix}
a_{11} & \cdots & a_{1n} \\
\vdots & \ddots & \vdots \\
a_{k1} & \cdots & a_{kn} \\
1 & \cdots & 1
\end{pmatrix}
\begin{pmatrix}
p \\
\vdots \\
p
\end{pmatrix}
= 
\begin{pmatrix}
b_1 \\
\vdots \\
b_k
\end{pmatrix} 
\iff
\mathbf{A} p = \mathbf{b}
\end{align*}
\]

• Entropy maximized subject to the equality constraints

\[
O(p, \mu) = H(p) + \mu'(\mathbf{A} p - \mathbf{b})
\]

\[
\begin{align*}
\frac{\partial O(p, \mu)}{\partial p} &= -\ln p - 1 + \mathbf{A}' \mu = 0 \\
\frac{\partial O(p, \mu)}{\partial \mu} &= \mathbf{A} p - \mathbf{b} = 0
\end{align*}
\]

\[
\iff
\begin{pmatrix}
0 & \mathbf{A}' \\
\mathbf{A} & 0
\end{pmatrix}
\begin{pmatrix}
p \\
\mu
\end{pmatrix}
= 
\begin{pmatrix}
\ln p + 1 \\
\mathbf{b}
\end{pmatrix}
\]

⇒ Sequence of MinNorm problems for solving the MaxEnt problem
MinNorm as an approximation of MaxEnt
MinNorm as an approximation of MaxEnt

- Taylor series of \( \ln p_i \) around \( p_i = k_i \)

\[
\ln p_i = \ln k_i + \sum_{j=1}^{\infty} (-1)^{j+1} \frac{1}{j k_i^j} (p_i - k_i)^j = \frac{p_i}{k_i} - 1 + \ln k_i + R_1(k_i)
\]
MinNorm as an approximation of MaxEnt

• Taylor series of \( \ln p_i \) around \( p_i = k_i \)

\[
\ln p_i = \ln k_i + \sum_{j=1}^{\infty} (-1)^{j+1} \frac{1}{jk_i^j} (p_i - k_i)^j = \frac{p_i}{k_i} - 1 + \ln k_i + R_1(k_i)
\]

• Truncating at degree one and summing over \( i \)

\[
- \sum_{i=1}^{n} p_i \ln p_i \approx - \sum_{i=1}^{n} \frac{p_i^2}{k_i} + \sum_{i=1}^{n} p_i - \sum_{i=1}^{n} p_i \ln k_i
\]

\[
= - \sum_{i=1}^{n} \frac{p_i^2}{k_i} - \sum_{i=1}^{n} p_i \ln k_i + 1
\]
MinNorm as an approximation of MaxEnt

• Taylor series of $\ln p_i$ around $p_i = k_i$

$$
\ln p_i = \ln k_i + \sum_{j=1}^{\infty} (-1)^{j+1} \frac{1}{jk_i^j} (p_i - k_i)^j = \frac{p_i}{k_i} - 1 + \ln k_i + R_1(k_i)
$$

• Truncating at degree one and summing over $i$

$$
- \sum_{i=1}^{n} p_i \ln p_i \simeq - \sum_{i=1}^{n} \frac{p_i^2}{k_i} + \sum_{i=1}^{n} p_i - \sum_{i=1}^{n} p_i \ln k_i
$$

$$
= - \sum_{i=1}^{n} \frac{p_i^2}{k_i} - \sum_{i=1}^{n} p_i \ln k_i + 1
$$

• In particular, if $k_i = 1/n$

$$
H(p) \simeq -n||p|| + \ln n + 1
$$
MinNorm as an approximation of MaxEnt

For any other choice of the $k_i$’s, by completing the square

$$p_i \ln p_i \simeq \frac{p_i^2}{k_i} + p_i \ln k_i - p_i$$

$$= \left( \frac{p_i}{\sqrt{k_i}} + \frac{1}{2} \sqrt{k_i \ln k_i} \right)^2 - \frac{1}{4} k_i \ln^2 k_i - p_i$$
MinNorm as an approximation of MaxEnt

- For any other choice of the $k_i$'s, by completing the square

$$p_i \ln p_i \simeq \frac{p_i^2}{k_i} + p_i \ln k_i - p_i$$

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- Summing over $i$

$$H(p) \simeq -||\tilde{p}|| + c$$

Where

$$\tilde{p} = (\tilde{p}_1, \ldots, \tilde{p}_n)'$$

$$\tilde{p}_i = \frac{p_i}{\sqrt{k_i}} + \frac{1}{2} \sqrt{k_i} \ln k_i$$

$$c = \frac{1}{4} \sum_{i=1}^{n} k_i \ln^2 k_i + 1$$
The MinDiv problem
The MinDiv problem

• Divergence or Kullback-Leibler distance

\[
D(p|q) = \sum_{i=1}^{n} p_i \ln \frac{p_i}{q_i} = p' \ln \left( \frac{[p]}{[q]} \right)
\]

with

\[
\begin{align*}
D(p|q) &\geq 0 \quad \forall (p, q) \\
D(p|q) = 0 &\iff p = q
\end{align*}
\]
The MinDiv problem

- Divergence or Kullback-Leibler distance

\[ D(p||q) = \sum_{i=1}^{n} p_i \ln \frac{p_i}{q_i} = p' \ln \left( \frac{[p]}{[q]} \right) \]

with \( \begin{cases} D(p||q) \geq 0 \quad \forall (p,q) \\ D(p||q) = 0 \iff p = q \end{cases} \)

- Equality constraints

\[ D(p||q) = 0 \iff \text{Maximizing} \quad H(p) \]
The MinDiv problem

• Divergence or Kullback-Leibler distance

\[ D(p||q) = \sum_{i=1}^{n} p_i \ln \frac{p_i}{q_i} = p' \ln \left( \frac{[p]}{[q]} \right) \]

with \[ \left\{ \begin{array}{c} D(p||q) \geq 0 \quad \forall (p,q) \\ D(p||q) = 0 \iff p = q \end{array} \right. \]

• Equality constraints

\[ D(p||q) = 0 \iff \text{Maximizing } H(p) \]

• Inequality constraints \( \Rightarrow \) Random vector Q
The MinDiv problem

• Divergence or Kullback-Leibler distance
\[ D(p||q) = \sum_{i=1}^{n} p_i \ln \frac{p_i}{q_i} = p' \ln \left( \frac{p}{q} \right) \]
with \[ \begin{cases} D(p||q) \geq 0 & \forall (p, q) \\ D(p||q) = 0 \iff p = q \end{cases} \]

• Equality constraints
\[ D(p||q) = 0 \iff \text{Maximizing} \quad H(p) \]

• Inequality constraints \( \Rightarrow \) Random vector \( Q \)
\( \Rightarrow \) Minimizing the expected divergence
\[ E[D(p||Q)] = -H(p) - p'E[\ln Q] \geq 0 \]
The MinDiv problem

- Divergence or Kullback-Leibler distance

\[ D(p||q) = \sum_{i=1}^{n} p_i \ln \frac{p_i}{q_i} = p' \ln \left( \left[ \frac{p}{q} \right] \right) \]

with \( \begin{cases} 
D(p||q) \geq 0 & \forall (p,q) \\
D(p||q) = 0 & \iff p = q 
\end{cases} \)

- Equality constraints

\[ D(p||q) = 0 \iff \text{Maximizing} \ H(p) \]

- Inequality constraints \( \Rightarrow \) Random vector Q

\( \Rightarrow \) Minimizing the expected divergence

\[ E[D(p||Q)] = -H(p) - p'E[\ln Q] \geq 0 \]

\( \Rightarrow \) Sequence of MinNorm problems for solving the MinDiv problem
The MinDiv problem

• Divergence or Kullback-Leibler distance
  \[ D(p||q) = \sum_{i=1}^{n} p_i \ln \frac{p_i}{q_i} = p' \ln \left( \frac{[p]}{[q]} \right) \]
  with \( \begin{cases} D(p||q) \geq 0 & \forall (p, q) \\ D(p||q) = 0 \iff p = q \end{cases} \)

• Equality constraints
  \[ D(p||q) = 0 \iff \text{Maximizing } H(p) \]

• Inequality constraints \( \Rightarrow \) Random vector Q
  \( \Rightarrow \) Minimizing the expected divergence
  \[ E[D(p||Q)] = -H(p) - p' E[\ln Q] \geq 0 \]

\( \Rightarrow \) Sequence of MinNorm problems for solving the MinDiv problem

Both **Equality** and **Inequality** constraints can be processed together by MinNorm approximations
MinNorm as an approximation of MinDiv
MinNorm as an approximation of MinDiv

- Taylor series around $p_i = k_i$ and completing the square

\[
p_i \ln p_i - p_i E[\ln Q_i] \simeq \frac{p_i^2}{k_i} + p_i (\ln k_i - E[\ln Q_i]) - p_i
\]

\[
= \left( \frac{p_i}{\sqrt{k_i}} + \frac{1}{2} \sqrt{k_i} (\ln k_i - E[\ln Q_i]) \right)^2
- \frac{1}{4} k_i \left( \ln k_i - E[\ln Q_i] \right)^2 - p_i
\]
MinNorm as an approximation of MinDiv

• Taylor series around $p_i = k_i$ and completing the square

\[
    p_i \ln p_i - p_i E[\ln Q_i] \simeq \frac{p_i^2}{k_i} + p_i (\ln k_i - E[\ln Q_i]) - p_i
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\[
    = \left( \frac{p_i}{\sqrt{k_i}} + \frac{1}{2} \sqrt{k_i} (\ln k_i - E[\ln Q_i]) \right)^2
    - \frac{1}{4} k_i (\ln k_i - E[\ln Q_i])^2 - p_i
\]

• Summing over $i$

\[
    E[D(p||Q)] \simeq ||\tilde{p}|| - c
\]

Where

\[
    \tilde{p} = (\tilde{p}_1, \ldots, \tilde{p}_n)'
    \tilde{p}_i = \frac{p_i}{\sqrt{k_i}} + \frac{1}{2} \sqrt{k_i} (\ln k_i - E[\ln Q_i])
\]

\[
    c = \frac{1}{4} \sum_{i=1}^n k_i (\ln k_i - E[\ln Q_i])^2 + 1
\]
Application in drainage classes mapping
Application in drainage classes mapping

• Categorical data are found in a wide variety of applications
Application in drainage classes mapping

- Categorical data are found in a wide variety of applications
- 90% of variables collected in soil surveys are categorical
Application in drainage classes mapping

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• Soil drainage, an important criterion in rating soils for various uses
Application in drainage classes mapping

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- 90% of variables collected in soil surveys are categorical
- Soil drainage, an important criterion in rating soils for various uses
- However, mapping methods ⇒ Laborious ⇒ Expensive
Application in drainage classes mapping

• Categorical data are found in a wide variety of applications

• 90% of variables collected in soil surveys are categorical

• Soil drainage, an important criterion in rating soils for various uses

• However, mapping methods ⇒ Laborious
  ⇒ Expensive

• Useful to integrate secondary information to improve the prediction
Application in drainage classes mapping

• Categorical data are found in a wide variety of applications

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• Soil drainage, an important criterion in rating soils for various uses

• However, mapping methods ⇒ Laborious
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• Useful to integrate secondary information to improve the prediction

⇒ Equality /Inequality information to improve the prediction
⇒ MinNorm approximations can deal with mathematical coding
Application in drainage classes mapping

- Belgian Lorraine, in the south of Luxembourg province

- Two information sources ⏪ 428 point observations of drainage classes
  ⏪ A lithological map as secondary information
Application in drainage classes mapping

- Belgian Lorraine, in the south of Luxembourg province
- Two information sources $\Rightarrow$ 428 point observations of drainage classes
  $\Rightarrow$ A lithological map as secondary information
Application in drainage classes mapping

\[ \hat{P}(D=c_i | L=c_j) \ [\%] \]

<table>
<thead>
<tr>
<th></th>
<th>j=1</th>
<th>j=2</th>
<th>j=3</th>
<th>j=4</th>
<th>j=5</th>
<th>j=6</th>
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<tr>
<td>i=1</td>
<td>55.6</td>
<td>62.7</td>
<td>22.2</td>
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<td>67.0</td>
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<td>31.9</td>
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Application in drainage classes mapping

\[ \hat{P}(D=c_i | L=c_j) \] [%]

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<tr>
<td>i=1</td>
<td>AMO</td>
<td>LUX</td>
<td>GRT</td>
<td>ETH</td>
<td>MIR</td>
<td>LGW</td>
</tr>
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Integrating the lithological map : 4 cases

- 4 cases for coding $P_{i|j} = P(\text{Drainage}=c_j | \text{Lithology}=c_j)$

<table>
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<tr>
<th>Case 1</th>
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<th>Case 4</th>
</tr>
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<tbody>
<tr>
<td>$P_{1</td>
<td>1} = 55.6$; $P_{2</td>
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<td>1} = 0.0$</td>
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<tr>
<td>$P_{1</td>
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</tr>
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<td>$P_{1</td>
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</tr>
<tr>
<td>$P_{1</td>
<td>4} = 28.1$; $P_{2</td>
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</tr>
<tr>
<td>$P_{1</td>
<td>5} = 78.6$; $P_{2</td>
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<td>5} = 7.1$</td>
</tr>
<tr>
<td>$P_{1</td>
<td>6} = 67.0$; $P_{2</td>
<td>6} = 31.9$; $P_{3</td>
<td>6} = 1.1$</td>
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- Information content degraded from case 1 to case 4
Integrating the lithological map : 4 cases

- 4 cases for coding $P_{i|j} = P(\text{Drainage}=c_j \mid \text{Lithology}=c_i)$

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<tr>
<td></td>
<td>(\hat{p}(D=c_i</td>
<td>L=c_j)) [%]</td>
<td></td>
<td></td>
</tr>
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<td></td>
<td>(j=1)</td>
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<tr>
<td>(i=1)</td>
<td>AMO: 55.6</td>
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**Notes:**
- \(D\) represents depth, \(L\) represents lithology, \(c_i\) and \(c_j\) are categories.
- The table shows the estimated probability \(\hat{p}(D=c_i|L=c_j)\) in percentage for each combination of depth and lithology categories in the four cases.
Spatial prediction
Integrating the lithological map: 4 cases

| Case 1 | \( \hat{P}(D=c_i|L=c_j) \) [%] |
|--------|-------------------------------|
|        | j=1 AMO | j=2 LUX | j=3 GRT | j=4 ETH | j=5 MIR | j=6 LGW |
| i=1    | 55.6     | 62.7    | 22.2    | 28.1    | 78.6    | 67.0    |
| i=2    | 44.4     | 34.9    | 66.7    | 61.4    | 14.3    | 31.9    |
| i=3    | 0.0      | 2.4     | 11.1    | 10.5    | 7.1     | 1.1     |

| Case 2 |            |            |
|--------|------------|
| j=1 AMO | j=2 LUX | j=3 GRT | j=4 ETH | j=5 MIR | j=6 LGW |
| i=1    | 45.7     | 64.6    | 15.7    | 15.7    | 68.5    | 67.9    |
| i=2    | 45.5     | 27.3    | 68.5    | 68.5    | 15.8    | 31.0    |
| i=3    | 8.8      | 8.1     | 15.7    | 15.7    | 15.7    | 1.1     |

| Case 3 |            |            |
|--------|------------|
| j=1 AMO | j=2 LUX | j=3 GRT | j=4 ETH | j=5 MIR | j=6 LGW |
| i=1    | 64.6     | 64.7    | 27.3    | 27.3    | 64.7    | 64.5    |
| i=2    | 27.3     | 27.3    | 64.6    | 64.7    | 27.3    | 27.4    |
| i=3    | 8.1      | 8.1     | 8.1     | 8.1     | 8.0     | 8.1     |

| Case 4 |            |            |
|--------|------------|
| j=1 AMO | j=2 LUX | j=3 GRT | j=4 ETH | j=5 MIR | j=6 LGW |
| i=1    | 68.4     | 68.5    | 15.8    | 15.7    | 68.6    | 68.5    |
| i=2    | 15.8     | 15.7    | 68.5    | 68.5    | 15.7    | 15.7    |
| i=3    | 15.8     | 15.8    | 15.8    | 15.8    | 15.7    | 15.9    |
Spatial prediction
Integrating the lithological map : 4 cases

\[ \hat{P}(D=c_i | L=c_j) \ ] \ [%]\]

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Conclusions
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- Equality $\Rightarrow$ MaxEnt
- Inequality $\Rightarrow$ MinDiv
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$\Rightarrow$ MinNorm Approximations
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• Approximations close to direct estimates when large amount of data
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\[\Rightarrow\quad \text{MinNorm Approximations}\]

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• In most cases in environmental sciences, \textbf{few data} are at hand
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$\Rightarrow$ Useful to integrate experts opinion
Thank you for your attention
References