# Bayesian statistics, Occam razor, and model-independent learning of continuous probability densities 

Ilya Nemenman<br>ITP, UCSB<br>Joint work with:<br>William Bialek, Princeton University

## Bayesian statistics ...

This is how it compares to other ultimate answers:

## Bayesian statistics ...

... claims that the the answer to the Great Question of Life, The Universe and Everything is not 42, but

This is how it compares to other ultimate answers:

## Bayesian statistics ...

... claims that the the answer to the Great Question of Life, The Universe and Everything is not 42, but

$$
P(\text { Model } \mid \text { Data })=\frac{P(\text { Data } \mid \text { Model }) \mathcal{P}(\text { Model })}{P(\text { Data })}
$$

This is how it compares to other ultimate answers:

## Bayesian statistics ...

... claims that the the answer to the Great Question of Life, The Universe and Everything is not 42, but

$$
P(\text { Model } \mid \text { Data })=\frac{P(\text { Data } \mid \text { Model }) \mathcal{P}(\text { Model })}{P(\text { Data })}
$$

This is how it compares to other ultimate answers:

## Bayes Best others

|  | Bayes | Best others |
| :--- | :---: | :---: |
| consistency | $\checkmark$ | $\checkmark$ |
| convergence rates | optimal | optimal |
| model selection | $?$ | $\checkmark$ (disagreement remains) |
| use of prior knowledge | $\checkmark$ | $?$ |

## Bayes Best others

model selection use of prior knowledge

## $\checkmark$ (disagreement remains)

?
later

## Bayes Best others

## model selection

?
today

## Bayesian model selection for finitely parameterizable distributions

# Bayesian model selection for finitely parameterizable distributions 

$P(x)$<br>unknown

## Bayesian model selection for finitely parameterizable distributions

$$
P(x) \xrightarrow{\text { i.i.d. }} X=\left\{x_{1} \cdots x_{N}\right\}
$$

## Bayesian model selection for finitely parameterizable distributions

$$
P(x) \xrightarrow{\text { i.i.d. }} X=\left\{x_{1} \cdots x_{N}\right\}
$$

```
    Model family A
        QA(x|\alpha)
    \operatorname{dim}\alpha=\mp@subsup{K}{A}{}
P
```


## Bayesian model selection for finitely parameterizable distributions

$$
P(x) \xrightarrow{\text { i.i.d. }} X=\left\{x_{1} \cdots x_{N}\right\}
$$

> Model family $A$
> $Q_{A}(x \mid \boldsymbol{\alpha})$
> $\operatorname{dim} \boldsymbol{\alpha}=K_{A}$
> $\mathcal{P}_{A}(\boldsymbol{\alpha}), \operatorname{Pr}(A)$

Model family $B$

$$
\begin{gathered}
Q_{B}(x \mid \boldsymbol{\beta}) \\
\operatorname{dim} \boldsymbol{\beta}=K_{B} \\
\mathcal{P}_{B}(\boldsymbol{\beta}), \operatorname{Pr}(B)
\end{gathered}
$$

## Bayesian model selection for finitely parameterizable distributions



Model family $A$

$$
\begin{gathered}
Q_{A}(x \mid \boldsymbol{\alpha}) \\
\operatorname{dim} \boldsymbol{\alpha}=K_{A} \\
\mathcal{P}_{A}(\boldsymbol{\alpha}), \operatorname{Pr}(A)
\end{gathered}
$$

Model family $B$

$$
\begin{gathered}
Q_{B}(x \mid \boldsymbol{\beta}) \\
\operatorname{dim} \boldsymbol{\beta}=K_{B} \\
\mathcal{P}_{B}(\boldsymbol{\beta}), \operatorname{Pr}(B)
\end{gathered}
$$

## Solution

## Find the model with maximum posterior probability!

## Solution

## Find the model with maximum posterior probability!

For example, for model $A$ :

$$
\begin{aligned}
& P(A \mid X)=\frac{P(X \mid A) \operatorname{Pr}(A)}{P(X)} P(X \mid A) \operatorname{Pr}(A)+P(X \mid B) \operatorname{Pr}(B)=Z \\
& P(X \mid A)=\int d \boldsymbol{\alpha} \mathcal{P}_{A}(\boldsymbol{\alpha}) P(X \mid \boldsymbol{\alpha}) \sim P\left(X \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)\left\|\delta \boldsymbol{\alpha}_{\mathrm{ML}}\right\|
\end{aligned}
$$

## Solution

## Find the model with maximum posterior probability!

For example, for model $A$ :

$$
\begin{aligned}
& P(A \mid X)=\frac{P(X \mid A) \operatorname{Pr}(A)}{P(X)} P(X \mid A) \operatorname{Pr}(A)+P(X \mid B) \operatorname{Pr}(B)=Z \\
& P(X \mid A)=\int d \boldsymbol{\alpha} \mathcal{P}_{A}(\boldsymbol{\alpha}) P(X \mid \boldsymbol{\alpha}) \sim P\left(X \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)\left\|\delta \boldsymbol{\alpha}_{\mathrm{ML}}\right\|
\end{aligned}
$$

For large $K_{A}, \delta \alpha_{M L}$ (region of "good" $\alpha$ ) decreases. More complicated models are penalized!

## Solution

## Find the model with maximum posterior probability!

For example, for model $A$ :

$$
\begin{aligned}
& P(A \mid X)=\frac{P(X \mid A) \operatorname{Pr}(A)}{P(X)} P(X \mid A) \operatorname{Pr}(A)+P(X \mid B) \operatorname{Pr}(B)=Z \\
& P(X \mid A)=\int d \boldsymbol{\alpha} \mathcal{P}_{A}(\boldsymbol{\alpha}) P(X \mid \boldsymbol{\alpha}) \sim P\left(X \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)\left\|\delta \boldsymbol{\alpha}_{\mathrm{ML}}\right\|
\end{aligned}
$$

For large $K_{A}, \delta \alpha_{M L}$ (region of "good" $\alpha$ ) decreases. More complicated models are penalized!

## Large $N$ expansion

## Saddle point (large $N$ ) expansion is almost always valid.

(See: Schwartz 1978, MacKay 1992, Balasubramanian 1996)

## Large $N$ expansion

Saddle point (large $N$ ) expansion is almost always valid.

$$
\log P(A \mid X) \rightarrow \sum_{i} \underbrace{\log Q_{A}\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}
$$

(See: Schwartz 1978, MacKay 1992, Balasubramanian 1996)

## Large $N$ expansion

Saddle point (large $N$ ) expansion is almost always valid.

$$
\begin{array}{rl}
\log P & P(A \mid X) \rightarrow \sum_{i} \underbrace{\log Q_{A}\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)} \\
& -\underbrace{\frac{K_{A}}{2} \log N-\log \operatorname{det} \partial^{2} \alpha_{\mathrm{ML}} \frac{\sum_{i} \log Q\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}{N}}
\end{array}
$$

(See: Schwartz 1978, MacKay 1992, Balasubramanian 1996)

## Large $N$ expansion

Saddle point (large $N$ ) expansion is almost always valid.

$$
\begin{aligned}
& \log P(A \mid X) \rightarrow \sum_{i} \underbrace{\log Q_{A}\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)} \\
& -\underbrace{\frac{K_{A}}{2} \log N-\log \operatorname{det} \partial_{\alpha_{\mathrm{ML}}}^{2} \frac{\sum_{i} \log Q\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}{N}} \\
& +\log \mathcal{P}\left(\boldsymbol{\alpha}_{\mathrm{ML}}\right)+o\left(N^{0}\right)
\end{aligned}
$$

(See: Schwartz 1978, MacKay 1992, Balasubramanian 1996)

## Large $N$ expansion

Saddle point (large $N$ ) expansion is almost always valid.

$$
\begin{aligned}
& \log P(A \mid X) \rightarrow \sum_{i} \underbrace{\log Q_{A}\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}_{\text {goodness of fit }} \\
& -\underbrace{-\underbrace{\frac{K_{A}}{2} \log N-\log \operatorname{det} \partial^{2} \alpha_{\mathrm{ML}} \frac{\sum_{i} \log Q\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}{N}}} \begin{aligned}
N
\end{aligned} \\
& \\
& \quad+\log \mathcal{P}\left(\boldsymbol{\alpha}_{\mathrm{ML}}\right)+o\left(N^{0}\right)
\end{aligned}
$$

(See: Schwartz 1978, MacKay 1992, Balasubramanian 1996)

## Large $N$ expansion

Saddle point (large $N$ ) expansion is almost always valid.

$$
\begin{aligned}
& \log P(A \mid X) \rightarrow \sum_{i} \underbrace{\log Q_{A}\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}_{\text {goodness of fit }} \\
& \\
& -\underbrace{\frac{K_{A}}{2} \log N-\log \operatorname{det} \partial^{2} \alpha_{\mathrm{ML}} \frac{\sum_{i} \log Q\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}{N}}
\end{aligned}
$$

generalization error, fluctuations, complexity; weak dependence on priors

$$
+\log \mathcal{P}\left(\boldsymbol{\alpha}_{\mathrm{ML}}\right)+o\left(N^{0}\right)
$$

(See: Schwartz 1978, MacKay 1992, Balasubramanian 1996)

## Large $N$ expansion

Saddle point (large $N$ ) expansion is almost always valid.

$$
\begin{aligned}
& \log P(A \mid X) \rightarrow \sum_{i} \underbrace{\log Q_{A}\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}_{\text {goodness of fit }} \\
& \\
& -\underbrace{\frac{K_{A}}{2} \log N-\log \operatorname{det} \partial^{2} \alpha_{\mathrm{ML}} \frac{\sum_{i} \log Q\left(x_{i} \mid \boldsymbol{\alpha}_{\mathrm{ML}}\right)}{N}}
\end{aligned}
$$

generalization error, fluctuations, complexity; weak dependence on priors

$$
+\log \mathcal{P}\left(\boldsymbol{\alpha}_{\mathrm{ML}}\right)+o\left(N^{0}\right)
$$

(See: Schwartz 1978, MacKay 1992, Balasubramanian 1996)

## Conclusions

## Conclusions

- Bayesian inference penalizes for complexity (large $K$ )


## Conclusions

- Bayesian inference penalizes for complexity (large $K$ )
- Fight between the goodness of fit and the complexity selects an optimal model family.


## Conclusions

- Bayesian inference penalizes for complexity (large K)
- Fight between the goodness of fit and the complexity selects an optimal model family.

This is a Bayesian analogue of the MDL principle.

## Conclusions

- Bayesian inference penalizes for complexity (large K)
- Fight between the goodness of fit and the complexity selects an optimal model family.

This is a Bayesian analogue of the MDL principle.

> Does this generalize to infinite-dimensional models?

## Estimating density

## Estimating density

## Standard setting (solving IE)

Fisher-Wald setting
(minimizing risk)

## Estimating density

## Standard setting

(solving IE)
$F(t)=\int_{-\infty}^{t} Q(x) d x$

Fisher-Wald setting
(minimizing risk)

$$
R[Q]=-\int_{-\infty}^{+\infty} \log Q(x) d F(x)
$$

## Estimating density

Standard setting
(solving IE)
$F(t)=\int_{-\infty}^{t} Q(x) d x$
$\frac{1}{N} \sum_{x_{i}} \Theta\left(x_{i}-t\right)=\int_{-\infty}^{t} Q(x) d x \quad R_{\mathrm{emp}}[Q]=-\sum_{x_{i}} \log Q\left(x_{i}\right)$

## Estimating density

Standard setting
(solving IE)
$F(t)=\int_{-\infty}^{t} Q(x) d x$
$\frac{1}{N} \sum_{x_{i}} \Theta\left(x_{i}-t\right)=\int_{-\infty}^{t} Q(x) d x \quad R_{\mathrm{emp}}[Q]=-\sum_{x_{i}} \log Q\left(x_{i}\right)$
Both settings hypersensitive to fluctuations in $F(t)$. Smoothing is required.

## Bayesian learning for $K \rightarrow \infty$

## Finite Infinite

## Bayesian learning for $K \rightarrow \infty$

| Finite | Infinite |
| :---: | :---: |
| $\alpha$ | $\phi(x)=-\log \ell_{0} Q(x)$ |

## Bayesian learning for $K \rightarrow \infty$

| Finite | Infinite |
| :---: | :---: |
| $\alpha$ | $\phi(x)=-\log \ell_{0} Q(x)$ |
| $\mathcal{P}(\alpha)$ | $\mathcal{P}[Q] \propto \exp [-\frac{\ell^{2 \eta-1}}{2} \underbrace{\int d x\left(\partial_{x}^{\eta} \phi\right)^{2}}$ |

## Bayesian learning for $K \rightarrow \infty$

| Finite | Infinite |
| :---: | :---: |
| $\boldsymbol{\alpha}$ | $\phi(x)=-\log \ell_{0} Q(x)$ |
| $\mathcal{P}(\boldsymbol{\alpha})$ | $\mathcal{P}[Q] \propto \underbrace{\exp [-\frac{\ell^{2 \eta-1}}{2} \underbrace{\int d x\left(\partial_{x}^{\eta} \phi\right)^{2}}_{\text {smoothness penalty }}]}$ |

## Bayesian learning for $K \rightarrow \infty$

| Finite | Infinite |
| :---: | :---: |
| $\boldsymbol{\alpha}$ | $\phi(x)=-\log \ell_{0} Q(x)$ |
| $\mathcal{P}(\boldsymbol{\alpha})$ | $\mathcal{P}[Q] \propto \underbrace{\exp [-\frac{\ell^{2 \eta-1}}{2} \underbrace{\int d d\left(\partial_{x}^{\eta} \phi\right)^{2}}_{\text {smoothes penalty }}]}_{\text {spline prior of order } 2 \eta-1}$ |

## Bayesian learning for $K \rightarrow \infty$

$\left.\begin{array}{|c|c|}\hline \text { Finite } & \text { Infinite } \\ \hline \boldsymbol{\alpha} & \phi(x)=-\log \ell_{0} Q(x) \\ \mathcal{P}(\boldsymbol{\alpha}) & \mathcal{P}[Q] \propto \exp [-\frac{\ell^{2 \eta-1}}{2} \underbrace{\int d x\left(\partial_{x}^{\eta} \phi\right)^{2}}_{\text {smoothness penalty }} \\ \left\{A, K_{A}\right\} & \{\ell, \eta(?)\} \text { - index continuum of families }\end{array}\right]$

## Bayesian learning for $K \rightarrow \infty$

| Finite | Infinite |
| :---: | :---: |
| $\alpha$ $\mathcal{P}(\boldsymbol{\alpha})$ | $\begin{gathered} \phi(x)=-\log \ell_{0} Q(x) \\ \mathcal{P}[Q] \propto \exp [-\frac{\ell^{2 \eta-1}}{2} \underbrace{\int d x\left(\partial_{x}^{\eta} \phi\right)^{2}}_{\text {smoothness penalty }}] \end{gathered}$ |
| $\begin{gathered} \left\{A, K_{A}\right\} \\ \operatorname{Pr}(A) \end{gathered}$ | spline prior of order $2 \eta-1$ $\{\ell, \eta(?)\}$ - index continuum of families $\operatorname{Pr}(\ell, \eta(?))$ |

## Bayesian learning for $K \rightarrow \infty$

| Finite | Infinite |
| :---: | :---: |
| $\alpha$ $\mathcal{P}(\boldsymbol{\alpha})$ | $\begin{gathered} \phi(x)=-\log \ell_{0} Q(x) \\ \mathcal{P}[Q] \propto \exp [-\frac{\ell^{2 \eta-1}}{2} \underbrace{\int d x\left(\partial_{x}^{\eta} \phi\right)^{2}}_{\text {smoothness penalty }}] \end{gathered}$ |
| $\begin{gathered} \left\{A, K_{A}\right\} \\ \operatorname{Pr}(A) \end{gathered}$ | spline prior of order $2 \eta-1$ $\{\ell, \eta(?)\}$ - index continuum of families $\operatorname{Pr}(\ell, \eta(?))$ |

(See: Bialek, Callan, Strong, 1996)

## Quantum Field Theory analogy

Fix $\ell$ and $\eta$ :

$$
=\frac{\left\langle Q(x) Q\left(x_{1}\right) \cdots Q\left(x_{N}\right)\right\rangle^{0}}{\underbrace{\left\langle Q\left(x_{1}\right) \cdots Q\left(x_{N}\right)\right\rangle^{0}}}
$$

Correlation function in a QFT
defined by $\mathcal{P}[Q]$

## Quantum Field Theory analogy

Fix $\ell$ and $\eta$ :

$$
P[Q \mid X]=\frac{P(X \mid Q) \mathcal{P}[Q]}{P(X)}
$$

$$
=\frac{\left\langle Q(x) Q\left(x_{1}\right) \cdots Q\left(x_{N}\right)\right\rangle^{0}}{\underbrace{\left\langle Q\left(x_{1}\right) \cdots Q\left(x_{N}\right)\right\rangle^{0}}}
$$

Correlation function in a QFT
defined by $\mathcal{P}[Q]$

## Quantum Field Theory analogy

Fix $\ell$ and $\eta$ :

$$
\begin{aligned}
P[Q \mid X] & =\frac{P(X \mid Q) \mathcal{P}[Q]}{P(X)} \\
\langle Q\rangle & =\frac{\int[d Q] \mathcal{P}[Q] Q(x) \prod_{i=1}^{N} Q\left(x_{i}\right)}{\int[d Q] P[Q] \prod_{i=1}^{N} Q\left(x_{i}\right)} \\
& =\frac{\left\langle Q(x) Q\left(x_{1}\right) \cdots Q\left(x_{N}\right)\right\rangle^{0}}{\left\langle Q\left(x_{1}\right) \cdots Q\left(x_{N}\right)\right\rangle^{0}}
\end{aligned}
$$

Correlation function in a QFT
defined by $\mathcal{P}[Q]$

## Explicit form of correlation functions

$$
\begin{aligned}
\text { C. F. } & \equiv \int[d Q] \mathcal{P}[Q] \prod_{i=1}^{N} Q\left(x_{i}\right) \\
& =\int[d \phi] \frac{1}{\ell_{0}^{N}} e^{-S[\phi]} \delta\left[\int d x \frac{1}{\ell_{0}} \mathrm{e}^{-\phi}-1\right] \\
\underbrace{S[\phi \phi]}_{\text {action }} & =\underbrace{\frac{\ell^{2 \eta-1}}{2} \int d x\left(\partial_{x}^{\eta} \phi\right)^{2}}_{\text {kinetic term }}+\underbrace{\sum_{i} \phi\left(x_{i}\right)}_{\text {random potential }}
\end{aligned}
$$

## Large $N$ approximation for $\eta=1$

ML (classical, saddle point) solution dominates

## Large $N$ approximation for $\eta=1$

ML (classical, saddle point) solution dominates

$$
\ell \partial_{x}^{2} \phi_{\mathrm{cl}}(x)+\frac{N}{\ell_{0}} \mathrm{e}^{-\phi_{\mathrm{cl}}(x)}=\sum_{j} \delta\left(x-x_{j}\right)
$$

## Large $N$ approximation for $\eta=1$

ML (classical, saddle point) solution dominates

$$
\begin{array}{cc}
\begin{array}{cc}
\text { converges to } \\
-\log \ell_{0} P(x)
\end{array} & \begin{array}{c}
\text { changes on scale } \\
\ell
\end{array} \\
\ell \partial_{x}^{2} \phi_{\mathrm{cl}}(x)+\frac{N}{\ell_{0}} \mathrm{e}^{-\phi_{\mathrm{cl}}(x)}=\sum_{j} \delta\left(x-x_{j}\right)
\end{array}
$$

## Large $N$ approximation for $\eta=1$

ML (classical, saddle point) solution dominates


$\begin{array}{cccccc}0_{0} & 0.2 & 0.4 & 0.6 & 0.8 & 1\end{array}$

## Large $N$ approximation for $\eta=1$, continued Van Vleck calculation of functional determinant:

## Large $N$ approximation for $\eta=1$, continued

 Van Vleck calculation of functional determinant:$$
\text { C. F. } \approx\left(1 / \ell_{0}\right)^{N} \mathrm{e}^{-S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}}(x)\right]}
$$

## Large $N$ approximation for $\eta=1$, continued

 Van Vleck calculation of functional determinant:$$
\begin{aligned}
\text { C. F. } & \approx\left(1 / \ell_{0}\right)^{N} \mathrm{e}^{-S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}}(x)\right]} \\
S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}]}\right. & =\underbrace{\frac{\ell}{2} \int d x\left(\partial \phi_{\mathrm{cl}}\right)^{2}}+\underbrace{\sum \phi_{\mathrm{cl}}\left(x_{i}\right)} \\
& +\underbrace{\frac{1}{2} \sqrt{\frac{N}{\ell \ell_{0}}} \int d x \mathrm{e}^{-\phi_{\mathrm{cl}}(x) / 2}}
\end{aligned}
$$

## Large $N$ approximation for $\eta=1$, continued

 Van Vleck calculation of functional determinant:$$
\begin{aligned}
\text { C. F. } & \approx\left(1 / \ell_{0}\right)^{N} \mathrm{e}^{-S_{\text {eff }}\left[\phi_{\mathrm{cl}}(x)\right]} \\
S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}}\right] & =\underbrace{\frac{\ell}{2} \int d x\left(\partial \phi_{\mathrm{cl}}\right)^{2}}_{\text {prior, smoothness }}+\underbrace{\sum \phi_{\mathrm{cl}}\left(x_{i}\right)}_{\text {goodness of fit }} \\
& +\underbrace{\frac{1}{2} \sqrt{\frac{N}{\ell \ell_{0}} \int d x \mathrm{e}^{-\phi_{\mathrm{cl}}(x) / 2}}}_{\text {fluctuations, complexity, error }}
\end{aligned}
$$

## How do we measure performance?

## How do we measure performance?

For $x \in[0, L)$ the universal learning curve is

$$
\Lambda(N) \rightarrow\left\langle D_{\mathrm{KL}}\left(P \| Q_{\mathrm{cl}}\right)\right\rangle_{\left\{x_{i}\right\}}^{0} \sim \sqrt{\frac{L}{\ell N}}
$$

## How do we measure performance?

For $x \in[0, L)$ the universal learning curve is

$$
\Lambda(N) \rightarrow\left\langle D_{\mathrm{KL}}\left(P \| Q_{\mathrm{cl}}\right)\right\rangle_{\left\{x_{i}\right\}}^{0} \sim \sqrt{\frac{L}{\ell N}}
$$

For a different $\eta$ :

$$
\Lambda(N) \sim\left(\frac{L}{\ell}\right)^{1 / 2 \eta} N^{1 / 2 \eta-1}
$$

## Learning curves for fixed $\ell, \eta=1$

## Learning curves for fixed $\ell, \eta=1$

## Learner's assumptions <br> $\mathcal{P}_{\ell, \eta=1}[Q]$

## Learning curves for fixed $\ell, \eta=1$

Learner's assumptions $\quad \mathcal{P}_{\ell, \eta=1}[Q]$
Actual target distribution $\mathcal{P}_{\ell_{a}, \eta_{a}}^{\prime}[Q]$

## Learning curves for fixed $\ell, \eta=1$

Learner's assumptions $\quad \mathcal{P}_{\ell, \eta=1}[Q]$
Actual target distribution $\mathcal{P}_{\ell_{a}, \eta_{a}}^{\prime}[Q]$
$\eta=\eta_{a}, \ell=\ell_{a} \quad$ learning typical cases, $\mathcal{P}=\mathcal{P}^{\prime}$

## Learning curves for fixed $\ell, \eta=1$

Learner's assumptions $\quad \mathcal{P}_{\ell, \eta=1}[Q]$
Actual target distribution $\mathcal{P}_{\ell_{a}, \eta_{a}}^{\prime}[Q]$
$\eta=\eta_{a}, \ell=\ell_{a} \quad$ learning typical cases, $\mathcal{P}=\mathcal{P}^{\prime}$
$\eta=\eta_{a}, \ell \neq \ell_{a} \quad$ marginal outliers of $\mathcal{P}$

## Learning curves for fixed $\ell, \eta=1$

Learner's assumptions $\quad \mathcal{P}_{\ell, \eta=1}[Q]$
Actual target distribution $\mathcal{P}_{\ell_{a}, \eta_{a}}^{\prime}[Q]$
$\eta=\eta_{a}, \ell=\ell_{a} \quad$ learning typical cases, $\mathcal{P}=\mathcal{P}^{\prime}$
$\eta=\eta_{a}, \ell \neq \ell_{a} \quad$ marginal outliers of $\mathcal{P}$
$\eta>\eta_{a}$
extremely rough outliers

## Learning curves for fixed $\ell, \eta=1$

Learner's assumptions $\quad \mathcal{P}_{\ell, \eta=1}[Q]$
Actual target distribution $\mathcal{P}_{\ell_{a}, \eta_{a}}^{\prime}[Q]$
$\eta=\eta_{a}, \ell=\ell_{a} \quad$ learning typical cases, $\mathcal{P}=\mathcal{P}^{\prime}$
$\eta=\eta_{a}, \ell \neq \ell_{a} \quad$ marginal outliers of $\mathcal{P}$
$\eta>\eta_{a}$
$\eta<\eta_{a}$
extremely rough outliers
extremely smooth outliers

## Learning curves for fixed $\ell, \eta=1$

Learner's assumptions
$\mathcal{P}_{\ell, \eta=1}[Q]$
Actual target distribution $\mathcal{P}_{\ell_{a}, \eta_{a}}^{\prime}[Q]$
$\eta=\eta_{a}, \ell=\ell_{a} \quad$ learning typical cases, $\mathcal{P}=\mathcal{P}^{\prime}$
$\eta=\eta_{a}, \ell \neq \ell_{a} \quad$ marginal outliers of $\mathcal{P}$
$\eta>\eta_{a}$
$\eta<\eta_{a}$
extremely rough outliers
extremely smooth outliers
Note: we must have $\eta>1 / 2$ for convergence of the integrals.

## Learning typical cases



$$
\begin{array}{ll}
\ell=0.4, & \Lambda=(0.54 \pm 0.07) N^{-0.483 \pm 0.014} \\
\ell=0.2, & \Lambda=(0.83 \pm 0.08) N^{-0.493 \pm 0.09} \\
\ell=0.05, & \Lambda=(1.64 \pm 0.16) N^{-0.507 \pm 0.09}
\end{array}
$$

## Learning marginal outliers



## Learning at $\ell=0.2$.

## Learning strong outliers



$$
\begin{array}{ll}
\eta_{a}=2, \ell_{a}=0.1, & \Lambda=(0.40 \pm 0.05) N^{-0.493 \pm 0.013} \\
\eta_{a}=0.8, \ell_{a}=0.1, & \Lambda=(1.06 \pm 0.08) N^{-0.355 \pm 0.008}
\end{array}
$$

## $\ell=0.1$ for $\eta_{a}=0$ and $\ell=0.2$ otherwise

## Conclusions for fixed $\eta$ and $\ell$



## Conclusions for fixed $\eta$ and $\ell$



## Conclusions for fixed $\eta$ and $\ell$



- No overfits!
b but suboptimal performance for learning outliers


## Smoothness scale selection

## Smoothness scale selection

Allow a prior over $\ell$, but keep $\eta=1$

$$
\text { C. F. } \rightarrow\langle\text { C. F. }\rangle_{\ell}
$$

## Smoothness scale selection

Allow a prior over $\ell$, but keep $\eta=1$

$$
\text { C. F. } \rightarrow\langle\mathrm{C} \cdot \mathrm{~F} \cdot\rangle_{\ell}=\int d \ell \operatorname{Pr}(\ell) \mathrm{e}^{-S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}}(\phi, \ell)\right]}
$$

## Smoothness scale selection

Allow a prior over $\ell$, but keep $\eta=1$

$$
\text { C. F. } \rightarrow\langle\mathrm{C} \cdot \mathrm{~F} \cdot\rangle_{\ell}=\int d \ell \operatorname{Pr}(\ell) \mathrm{e}^{-S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}}(\phi, \ell)\right]}
$$

$$
S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}]}\right]=\underbrace{\text { smoothing }+ \text { data }}+\underbrace{\text { fluctuations }}
$$

## Smoothness scale selection

Allow a prior over $\ell$, but keep $\eta=1$

$$
\begin{gathered}
\text { C. F. } \rightarrow\langle\text { C. F. }\rangle_{\ell}=\int d \ell \operatorname{Pr}(\ell) \mathrm{e}^{-S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}}(\phi, \ell)\right]} \\
S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}}\right]=\underbrace{\text { smoothing }+ \text { data }}_{\text {grows with } \ell}+\underbrace{\text { fluctuations }}_{\text {grows with } 1 / \ell}
\end{gathered}
$$

## Smoothness scale selection

Allow a prior over $\ell$, but keep $\eta=1$

$$
\begin{aligned}
& \text { C. F. } \rightarrow\langle\mathrm{C} . \mathrm{F} .\rangle_{\ell}=\int d \ell \operatorname{Pr}(\ell) \mathrm{e}^{-S_{\mathrm{eff}}\left[\phi_{\mathrm{cl}}(\phi, \ell)\right]} \\
& S_{\text {eff }}\left[\phi_{\mathrm{cl}}\right]=\underbrace{\text { smoothing }+ \text { data }}_{\text {grows with } \ell}+\underbrace{\text { fluctuations }}_{\text {grows with } 1 / \ell} \\
& \text { Some } \ell^{*} \text { always dominates the C. F. and }\langle Q\rangle!
\end{aligned}
$$

## Calculations: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?

## Averaging over $\ell$ and allowing $\ell^{*}=\ell^{*}(N)$ deals with

## Calculations: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?

$$
\text { If } \eta=\eta_{a} \text {, then } \ell^{*}=\ell_{a} \text {. }
$$

## Averaging over $\ell$ and allowing $\ell^{*}=\ell^{*}(N)$ deals with

## Calculations: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?

If $\eta=\eta_{a}$, then $\ell^{*}=\ell_{a}$. Otherwise:

$$
\begin{array}{l|l}
\hline 0.5<\eta_{a} \leq 1.5 & 1.5<\eta_{a} \\
\hline
\end{array}
$$

## Averaging over $\ell$ and allowing $\ell^{*}=\ell^{*}(N)$ deals with

## Calculations: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?

If $\eta=\eta_{a}$, then $\ell^{*}=\ell_{a}$. Otherwise:

| $0.5<\eta_{a} \leq 1.5$ | $1.5<\eta_{a}$ |
| :---: | :---: |
| data $>$ smoothing | smoothing $>$ data |

## Averaging over $\ell$ and allowing $\ell^{*}=\ell^{*}(N)$ deals with

## Calculations: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?

If $\eta=\eta_{a}$, then $\ell^{*}=\ell_{a}$. Otherwise:

| $0.5<\eta_{a} \leq 1.5$ | $1.5<\eta_{a}$ |
| :---: | :---: |
| data $>$ smoothing | smoothing $>$ data |
| $\ell^{*} \sim N^{\left(\eta_{a}-1\right) / \eta_{a}}$ | $\ell^{*} \sim N^{1 / 3}$ |

## Averaging over $\ell$ and allowing $\ell^{*}=\ell^{*}(N)$ deals with

## Calculations: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?

If $\eta=\eta_{a}$, then $\ell^{*}=\ell_{a}$. Otherwise:

| $0.5<\eta_{a} \leq 1.5$ | $1.5<\eta_{a}$ |
| :---: | :---: |
| data $>$ smoothing | smoothing $>$ data |
| $\ell^{*} \sim N^{\left(\eta_{a}-1\right) / \eta_{a}}$ | $\ell^{*} \sim N^{1 / 3}$ |
| $\Lambda \sim N^{1 / 2 \eta_{a}-1}$ | $\Lambda \sim N^{-2 / 3}$ |

## Averaging over $\ell$ and allowing $\ell^{*}=\ell^{*}(N)$ deals with

## Calculations: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?

If $\eta=\eta_{a}$, then $\ell^{*}=\ell_{a}$. Otherwise:

| $0.5<\eta_{a} \leq 1.5$ | $1.5<\eta_{a}$ |
| :---: | :---: |
| data $>$ smoothing | smoothing $>$ data |
| $\ell^{*} \sim N^{\left(\eta_{a}-1\right) / \eta_{a}}$ | $\ell^{*} \sim N^{1 / 3}$ |
| $\Lambda \sim N^{1 / 2 \eta_{a}-1}$ | $\Lambda \sim N^{-2 / 3}$ |
| best possible | better, but not |
| performance | best performance |

Averaging over $\ell$ and allowing $\ell^{*}=\ell^{*}(N)$ deals with

## qualitatively wrong smoothness $\eta_{a} \neq 1$ !

## Numerics: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?

## Numerics: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?



Note: just single runs shown.

## Numerics: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?



Note: just single runs shown.

## Numerics: What is $\ell^{*}$ for $\eta_{a}$ and $\ell_{a}$ ?



Note: just single runs shown.

## Approaching model-independend optimal inference!

## Analogies

## Analogies

- choosing $\ell^{*}$ corresponds to selection of a structure element with $d_{\mathrm{VC}}=\sqrt{N L / \ell^{*}}$ in Vapnik's SRM theory


## Analogies

- choosing $\ell^{*}$ corresponds to selection of a structure element with $d_{\mathrm{VC}}=\sqrt{N L / \ell^{*}}$ in Vapnik's SRM theory
- maximizing $P$ over model families ( $\ell$ 's) asymptotically corresponds to searching for MDL


## Analogies

- choosing $\ell^{*}$ corresponds to selection of a structure element with $d_{\mathrm{VC}}=\sqrt{N L / \ell^{*}}$ in Vapnik's SRM theory
- maximizing $P$ over model families ( $\ell$ 's) asymptotically corresponds to searching for MDL
- a lot in common with the Gaussian Processes theory; however normalization constraint is important


## Summary

## Bayesian smoothness (model) selection works for nonparametric spline priors!

## Open questions

## Open questions

constant factor or constant summand?

## Open questions

constant factor or constant summand?

- what to do with $\eta_{a}>1.5$ ?


## Open questions

constant factor or constant summand?

- what to do with $\eta_{a}>1.5$ ?
- reparameterization invariance


## Open questions

constant factor or constant summand?

- what to do with $\eta_{a}>1.5$ ?
- reparameterization invariance
- information theoretic meaningful priors


## Open questions

constant factor or constant summand?

- what to do with $\eta_{a}>1.5$ ?
- reparameterization invariance
- information theoretic meaningful priors
- higher dimensions


## Open questions

constant factor or constant summand?

- what to do with $\eta_{a}>1.5$ ?
- reparameterization invariance
- information theoretic meaningful priors
- higher dimensions
- smooth transition from $K=$ const to $K \rightarrow \infty$


## Open questions

- constant factor or constant summand?
- what to do with $\eta_{a}>1.5$ ?
- reparameterization invariance
- information theoretic meaningful priors
- higher dimensions
- smooth transition from $K=$ const to $K \rightarrow \infty$
- which classes of priors are allowed?


## Open questions

constant factor or constant summand?

- what to do with $\eta_{a}>1.5$ ?
- reparameterization invariance
- information theoretic meaningful priors
- higher dimensions
- smooth transition from $K=$ const to $K \rightarrow \infty$
- which classes of priors are allowed?

There is hope that all of this problems are resolvable in a single formulation.

