Occam factors, spline priors, and model-independent learning of continuous distributions

> Ilya Nemenman ITP, UCSB

Joint work with: William Bialek, Princeton University

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P(x)

$$P(x) \xrightarrow{\text{i.i.d.}} X = \{x_1 \cdots x_N\}$$

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unknown

Model family
$$A$$

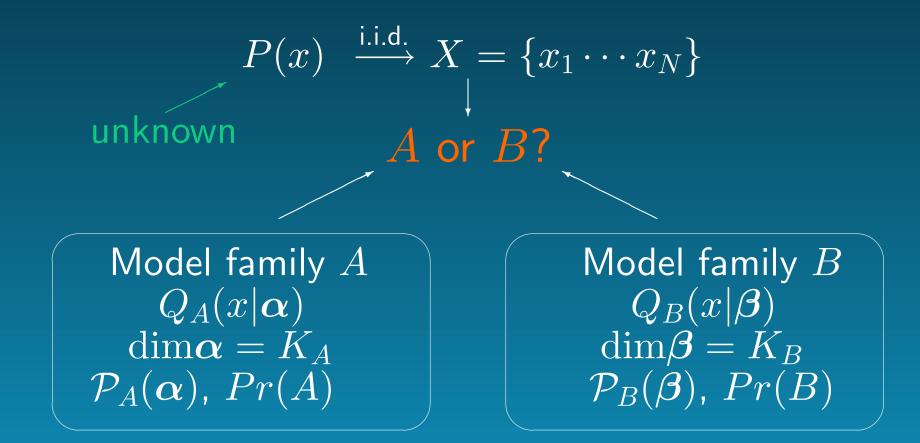
 $Q_A(x|\boldsymbol{\alpha})$
 $\dim \boldsymbol{\alpha} = K_A$
 $\mathcal{P}_A(\boldsymbol{\alpha}), Pr(A)$

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Model family A $Q_A(x|\boldsymbol{\alpha})$ $\dim \boldsymbol{\alpha} = K_A$ $\mathcal{P}_A(\boldsymbol{\alpha}), Pr(A)$ Model family B $Q_B(x|\beta)$ $\dim\beta = K_B$ $\mathcal{P}_B(\beta), Pr(B)$

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Find the model with maximum posterior probability!

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$$P(A|X) = \frac{P(X|A)Pr(A)}{P(X)} \xrightarrow{P(X|A)Pr(A) + P(X|B)Pr(B) \equiv Z}$$
$$P(X|A) = \int d\boldsymbol{\alpha} \mathcal{P}_A(\boldsymbol{\alpha}) P(X|\boldsymbol{\alpha}) \sim P(X|\boldsymbol{\alpha}_{\mathrm{ML}}) \,\delta\boldsymbol{\alpha}_{\mathrm{ML}}$$

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For large K_A , $\delta \alpha_{\rm ML}$ (region of "good" α) decreases. More complicated models are penalized!

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For large K_A , $\delta \alpha_{\rm ML}$ (region of "good" α) decreases. More complicated models are penalized! (See: Bayes factors, Occam factors; Jaynes 1968, 1979)

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

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

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generalization error, fluctuations, complexity; weak dependence on priors

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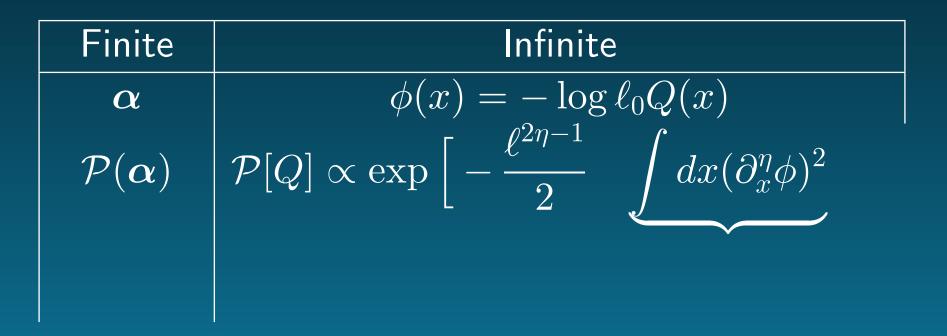
- Fight between the goodness of fit and the complexity selects an optimal model family.
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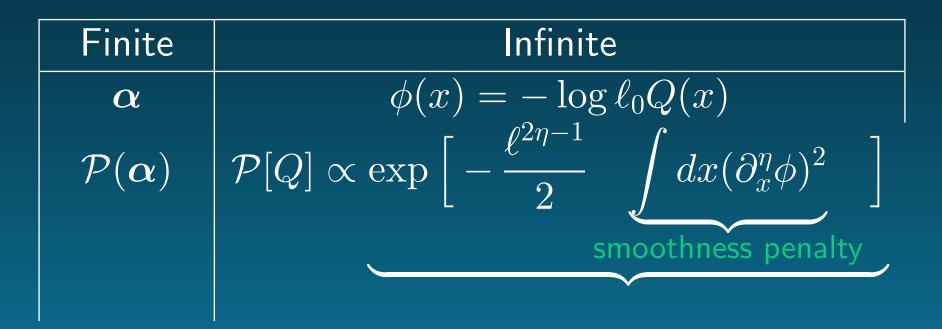
Does this generalize to infinite-dimensional models?

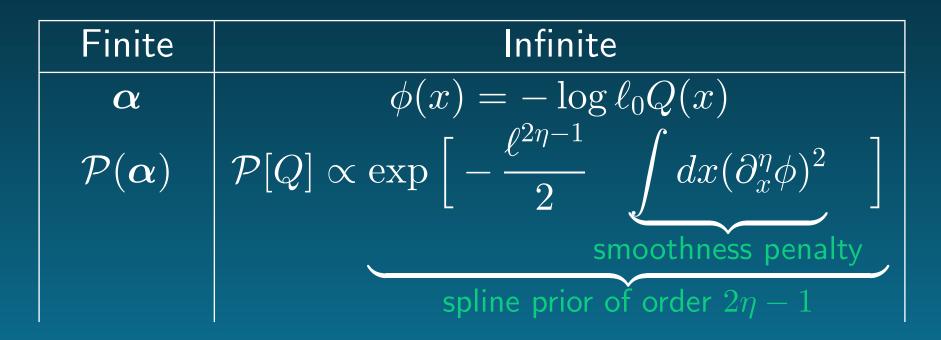
Finite Infinite	
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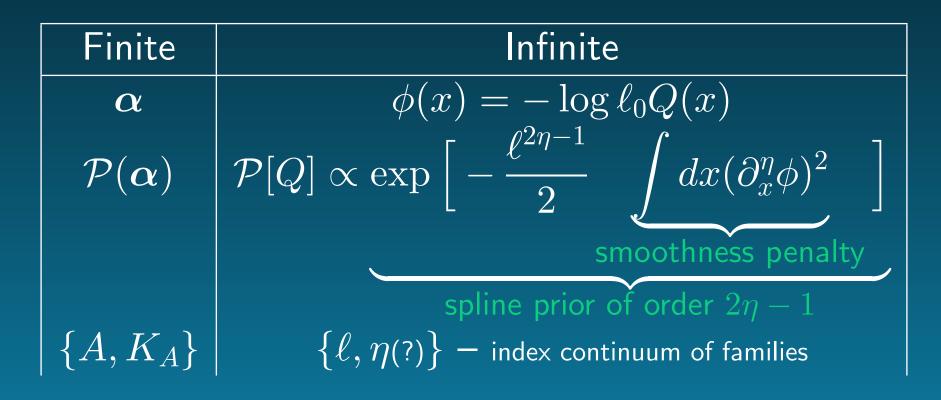
Finite	Infinite
α	$\phi(x) = -\log \ell_0 Q(x)$

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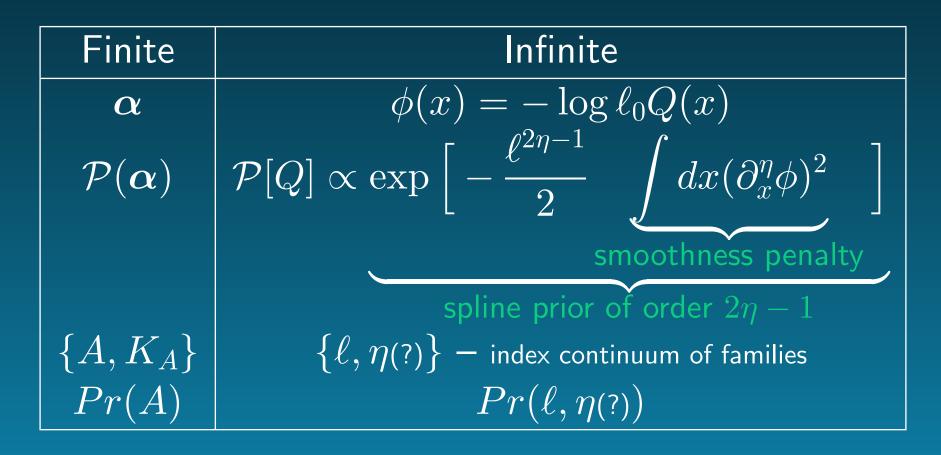


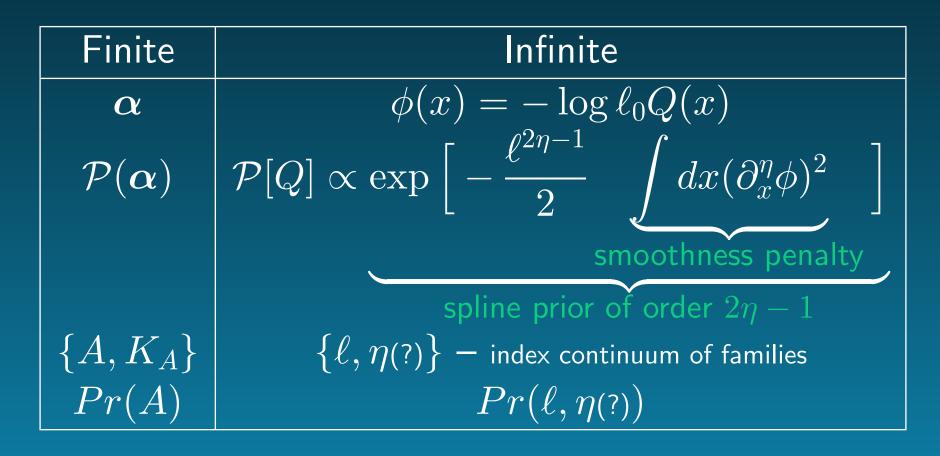






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(See: Bialek, Callan, Strong, 1996)

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Quantum Field Theory analogy Fix ℓ and η :

$$= \frac{\langle Q(x)Q(x_1)\cdots Q(x_N)\rangle^0}{\langle Q(x_1)\cdots Q(x_N)\rangle^0}$$

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

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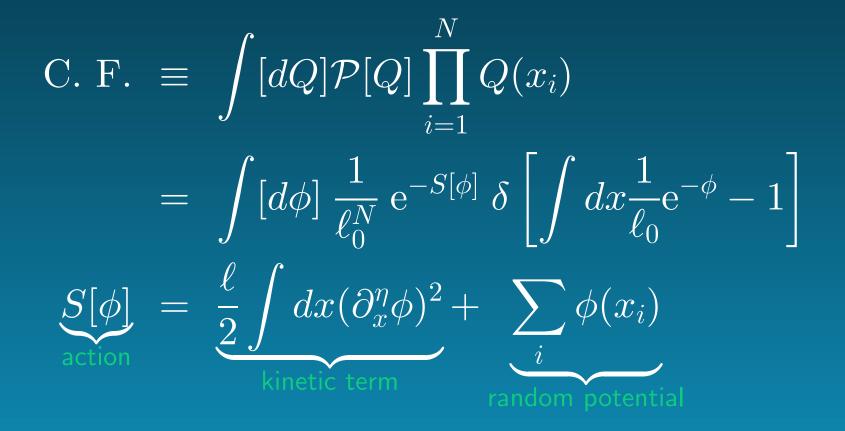
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Quantum Field Theory analogy Fix ℓ and η :

 $P[Q|X] = \frac{P(X|Q)\mathcal{P}[Q]}{P(X)}$ $\langle Q \rangle = \frac{\int [dQ] \mathcal{P}[Q] Q(x) \prod_{i=1}^{N} Q(x_i)}{\int [dQ] P[Q] \prod_{i=1}^{N} Q(x_i)}$ $= \frac{\langle Q(x)Q(x_1)\cdots Q(x_N)\rangle^0}{\langle Q(x_1)\cdots Q(x_N)\rangle^0}$

Correlation function in a QFT defined by $\mathcal{D}[O]$

Explicit form of correlation functions



Large N approximation for $\eta = 1$ ML (classical, saddle point) solution dominates

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$$\ell \partial_x^2 \phi_{\rm cl}(x) + \frac{N}{\ell_0} \mathrm{e}^{-\phi_{\rm cl}(x)} = \sum_j \delta(x - x_j)$$

Large N approximation for $\eta = 1$ ML (classical, saddle point) solution dominates

changes on scale converges to changes on scale $\delta x \sim \sqrt{\ell/NP(x)}$

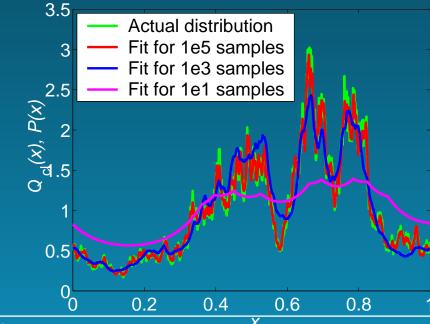
 $\frac{1}{\ell \partial_x^2 \phi_{\rm cl}(x)} + \frac{N}{\ell_0} e^{-\phi_{\rm cl}(x)} = \sum_j \delta(x - x_j)$

Large N approximation for $\eta = 1$ ML (classical, saddle point) solution dominates

 $-\log \ell_0 P(x)$ $\delta x \sim \sqrt{\ell/NP(x)}$

 $\ell \partial_x^2 \phi_{\rm cl}(x) + \frac{N}{\ell_0} \mathrm{e}^{-\phi_{\rm cl}(x)} = \sum_j \delta(x - x_j)$

changes on scale



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converges to

|C. F. $\approx (1/\ell_0)^N e^{-S_{\text{eff}}[\phi_{\text{cl}}(x)]}$

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back to start

C. F.
$$\approx (1/\ell_0)^N e^{-S_{\text{eff}}[\phi_{\text{cl}}(x)]}$$

 $S_{\text{eff}}[\phi_{\text{cl}}] = \frac{\ell}{2} \int dx (\partial \phi_{\text{cl}})^2 + \sum \phi_{\text{cl}}(x_i)$
 $+ \frac{1}{2} \sqrt{\frac{N}{\ell \ell_0}} \int dx e^{-\phi_{\text{cl}}(x)/2}$

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fluctuations, complexity, error

How do we measure performance?

How do we measure performance? For $x \in [0, L)$ the *universal* learning curve is $\Lambda(N) \rightarrow \langle D_{\mathrm{KL}}(P||Q_{\mathrm{cl}}) \rangle_{\{x_i\}}^0 \sim \sqrt{\frac{L}{\ell N}}$ How do we measure performance? For $x \in [0, L)$ the *universal* learning curve is $\Lambda(N) \rightarrow \langle D_{\mathrm{KL}}(P||Q_{\mathrm{cl}}) \rangle_{\{x_i\}}^0 \sim \sqrt{\frac{L}{\ell N}}$

For a different η :

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

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

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Learner's assumptions Actual target distribution

$$\mathcal{P}_{\ell,\eta=1}[Q] \\ \mathcal{P}'_{\ell_a,\eta_a}[Q]$$

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Learner's assumptions $\mathcal{P}_{\ell,\eta=1}[Q]$ Actual target distribution $\mathcal{P}'_{\ell_a,\eta_a}[Q]$ $\eta = \underline{\eta}_a, \ \ell = \ell_a$ learning typical cases, $\mathcal{P} = \mathcal{P}'$

Learner's assumptions $\mathcal{P}_{\ell,\eta=1}[Q]$ Actual target distribution $\mathcal{P}'_{\ell_a,\eta_a}[Q]$

 $\eta = \eta_a$, $\ell = \ell_a$ learning typical cases, $\mathcal{P} = \mathcal{P}'$ $\eta = \eta_a$, $\ell \neq \ell_a$ marginal outliers of \mathcal{P}

Learner's assumptions $\mathcal{P}_{\ell,\eta=1}[Q]$ Actual target distribution $\mathcal{P}'_{\ell_a,\eta_a}[Q]$

$$\begin{split} \eta &= \eta_a, \ \ell = \ell_a & \text{learning typical cases, } \mathcal{P} = \mathcal{P}' \\ \eta &= \eta_a, \ \ell \neq \ell_a & \text{marginal outliers of } \mathcal{P} \\ \eta &> \eta_a & \text{extremely rough outliers} \end{split}$$

Learner's assumptions $\mathcal{P}_{\ell,\eta=1}[Q]$ Actual target distribution $\mathcal{P}'_{\ell_a,\eta_a}[Q]$

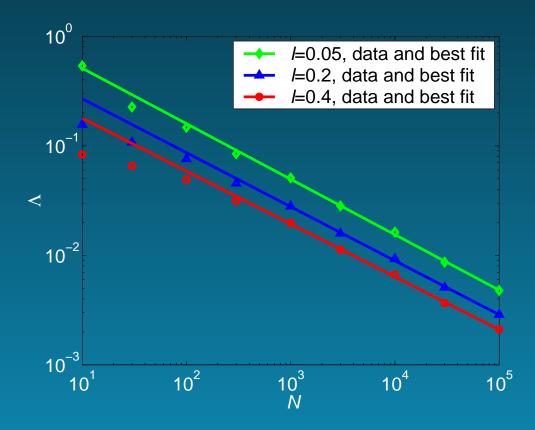
$\eta=\eta_a$, $\ell=\ell_a$	learning typical cases, $\mathcal{P} = \mathcal{P}'$
$\eta=\eta_a$, $\ell eq\ell_a$	marginal outliers of ${\cal P}$
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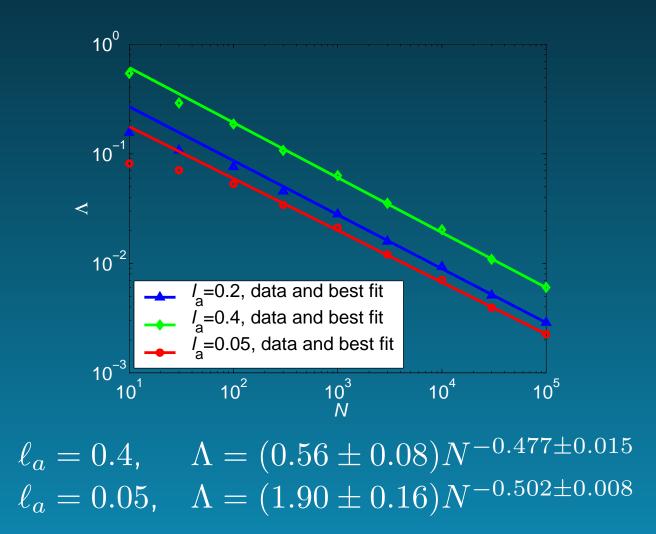
Note: we must have $\eta > 1/2$ for convergence of the integrals.

Learning typical cases



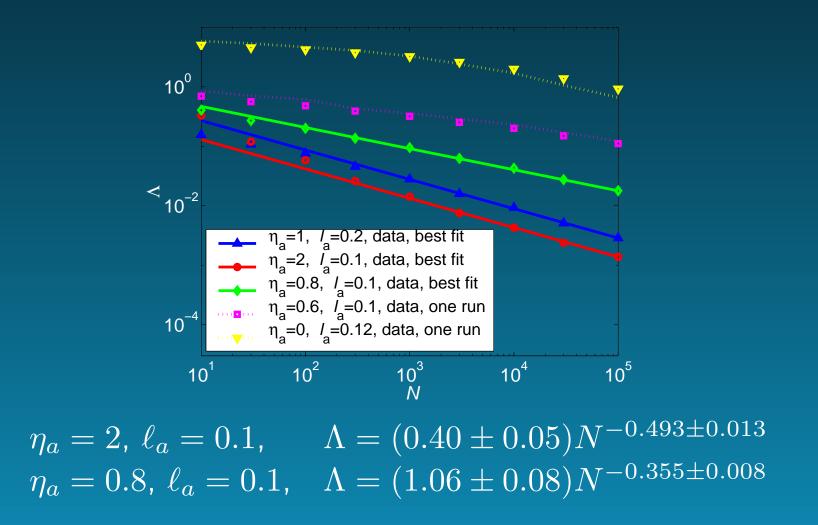
$$\begin{split} \ell &= 0.4, \quad \Lambda = (0.54 \pm 0.07) N^{-0.483 \pm 0.014} \\ \ell &= 0.2, \quad \Lambda = (0.83 \pm 0.08) N^{-0.493 \pm 0.09} \\ \ell &= 0.05, \quad \Lambda = (1.64 \pm 0.16) N^{-0.507 \pm 0.09} \end{split}$$

Learning marginal outliers



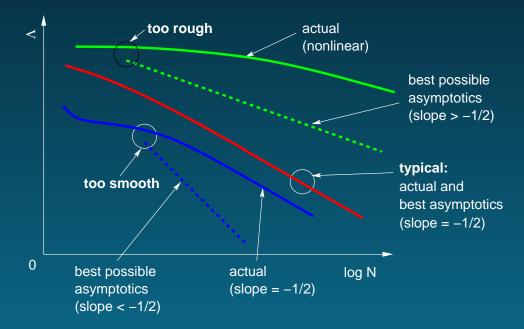
Learning at $\ell = 0.2$.

Learning strong outliers

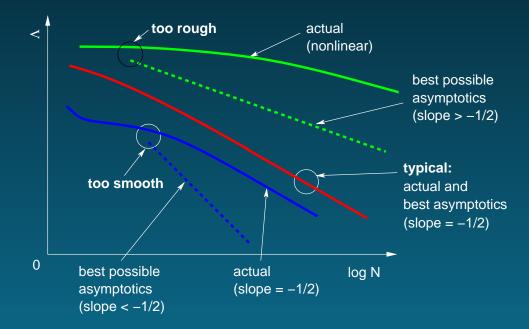


 $\ell = 0.1$ for $\eta_a = 0$ and $\ell = 0.2$ otherwise

Conclusions for fixed η and ℓ

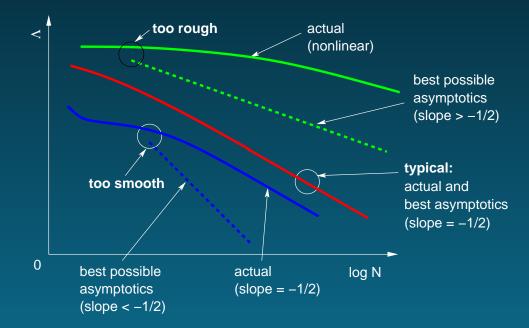


Conclusions for fixed η and ℓ



• No overfits!

Conclusions for fixed η and ℓ



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but suboptimal performance for learning outliers

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

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

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

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 $S_{\rm eff}[\phi_{\rm cl}] =$ smoothing + data + fluctuations

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m smoothing} + {
m data}_{
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m fluctuations}_{
m grows \ {
m with} \ \ell} \qquad {
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m with} \ 1/\ell}$$

Smoothness scale selection

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m grows with \ell} + {
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Some ℓ^* always dominates the C. F. and $\langle Q \rangle$!

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

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If $\eta = \eta_a$, then $\ell^* = \ell_a$.

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If $\eta = \eta_a$, then $\ell^* = \ell_a$. Otherwise:

$$0.5 < \eta_a \le 1.5 \qquad \qquad 1.5 < \eta_a$$

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data $>$ smoothing	smoothing > data

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If $\eta = \eta_a$, then $\ell^* = \ell_a$. Otherwise:

$$\begin{array}{ll} 0.5 < \eta_a \leq 1.5 & 1.5 < \eta_a \\ \mbox{data} > \mbox{smoothing} & \mbox{smoothing} > \mbox{data} \\ \ell^* \sim N^{(\eta_a - 1)/\eta_a} & \ell^* \sim N^{1/3} \end{array}$$

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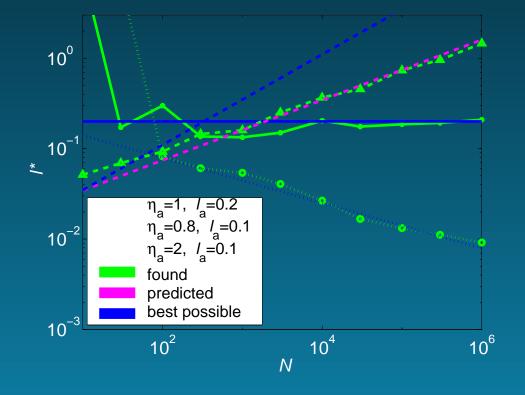
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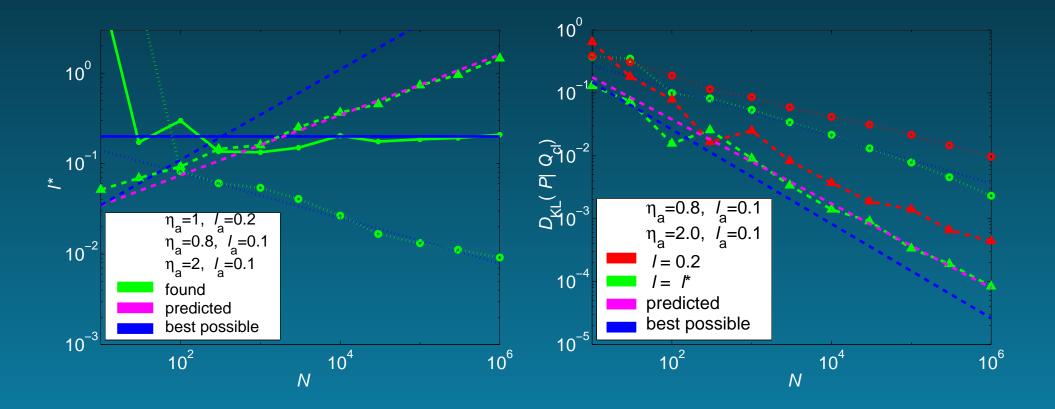
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data > smoothing	smoothing $>$ data
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$\Lambda \sim N^{1/2\eta_a - 1}$	$\Lambda \sim N^{-2/3}$
best possible	better, but not
performance	best performance

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

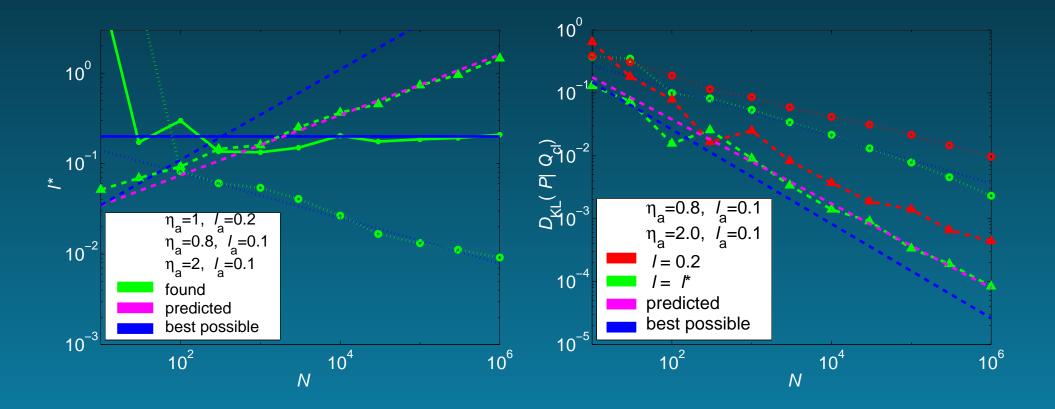
qualitatively wrong smoothness $\eta_a \neq 1!$



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Approaching model-independend optimal inference!

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

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 a lot in common with the Gaussian Processes theory; however normalization constraint is important 29

Summary

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

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