Prediction without probability: a PDE approach to a model problem from machine learning

Robert V. Kohn
Courant Institute, NYU

Joint work with Kangping Zhu (PhD 2014) and Nadejda Drenska (in progress)

Mathematics for Nonlinear Phenomena: Analysis and Computation
celebrating Yoshikazu Giga’s contributions and impact
Sapporo, August 2015
Looking back

We met in Tokyo in July 1982, at a US-Japan seminar. Giga came to Courant soon thereafter. We decided to study blowup of $u_t = \Delta u + u^p$. Over the next few years we had a lot of fun.

- Asymptotically self-similar blowup of semilinear heat equations, CPAM (1985)
- Characterizing blowup using similarity variables, IUMJ (1987)
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Over the years

Our paths have crossed many times, and in many ways.

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1983, Caffarelli-Kohn-Nirenberg: Partial regularity of suitable wk solns of the Navier-Stokes eqns

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Crystalline surface energies

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Many thanks for

- your huge impact on our field
- your leadership (both scientific and practical)
- helping our community grow and prosper
- a lot of fun in our joint projects
- your friendship over the years.
Today’s mathematical topic

Prediction without probability: a PDE approach to a model problem from machine learning

1. The problem (“prediction with expert advice”)
2. Two very simple experts
3. Two more realistic experts
4. Perspective
Basic idea: given

- a data stream
- a notion of prediction
- some experts

the overall goal is to beat the (retrospectively) best-performing expert – or at least, not do too much worse.

Jargon: minimize regret.

Widely-used paradigm in machine learning. Many variants, assoc to different types of data, classes of experts, notions of prediction.

Note analogy to a common business news feature . . .
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The stock prediction problem

A classic model problem (T Cover 1965, and many people since):

A stock goes up or down (data stream is binary, no probability)

- Investor buys (or sells) \( f \) shares of stock at each time step, \(|f| \leq 1\). Effectively, he is making a prediction.
- Two experts (to be specified soon). Regret wrt a given expert = (expert’s gain) - (investor’s gain).

Typical goal: minimize the worst-case value of regret wrt best-performing expert at a given future time \( T \).

More general goal: Minimize worst-case value of

\[ \phi(\text{regret wrt expert 1}, \text{regret wrt expert 2}) \]

at time \( T \). (The “typical goal” is \( \phi(x_1, x_2) = \max\{x_1, x_2\} \).)
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Very simple experts vs more realistic experts

Recall: stock goes up or down (data stream is binary, no probability)

- Investor buys (or sells) $f$ shares of stock at each time step, $|f| \leq 1$. Effectively, he is making a prediction.
- Two experts, each using a public algorithm to make his choice.

**First pass:** Two very simple experts – one always expects the stock to go up (he chooses $f = 1$), the other always expects the stock to go down (he chooses $f = -1$).

**Second pass:** Two more realistic experts – each looks at the last $d$ moves, and makes a choice depending on this recent history.

Essentially an optimal control problem:

- **state space**: \((x_1, x_2) = \text{relative regrets wrt + expert, relative regrets wrt - expert}\).
- **control**: investor’s stock purchase \(|f| \leq 1\).
- **value function**: \(v(x, t) = \text{optimal (worst-case) time-} T \text{ result, starting from relative regrets } x = (x_1, x_2) \text{ at time } t\).

**Dynamic programming principle**:

\[
v(x_1, x_2, t) = \min_{|f| \leq 1} \max_{b = \pm 1} v(\text{new position}, t + 1) \\
= \min_{|f| \leq 1} \max_{b = \pm 1} v(x_1 + b(1 - f), x_2 - b(1 + f), t + 1)
\]

for \(t < T\), with final-time condition \(v(x, T) = \phi(x)\).
Recall: \((x_1, x_2) = (\text{regret wrt } + \text{ expert, regret wrt } - \text{ expert}),\) where regret = (expert’s gain) - (investor’s gain).

If investor buys \(f\) shares and market goes up, investor gains \(f\), the + expert gains 1, the − expert gains −1. So state moves from \((x_1, x_2)\) to \((x_1 + (1 - f), x_2 + (-1 - f))\).

Similarly, if investor buys \(f\) shares and market goes down, state moves from \((x_1, x_2)\) to \((x_1 - (1 - f), x_2 - (-1 - f))\).

Hence the dynamic programming principle:

\[
v(x_1, x_2, t) = \min_{|f| \leq 1} \max_{b = \pm 1} v(\text{new position}, t + 1)
\]
\[
= \min_{|f| \leq 1} \max_{b = \pm 1} v(x_1 + b(1 - f), x_2 - b(1 + f), t + 1)
\]
In machine learning, one is interested in how regret accumulates over many time steps.

To access this question, it is natural to rescale the problem and look for a continuum limit.

Our problem has no probability. But our rescaling is like the passage from random walk to diffusion.

Our problem shares many features with the two-person-game interpretation of motion by curvature (work with Sylvia Serfaty, CPAM 2006).

So: consider a scaled version of problem: stock moves are $\pm \epsilon$ and time steps are $\epsilon^2$. The value function is still the optimal worst-case time-$T$ result. The principle of dynamic programming becomes

$$w^\epsilon(x_1, x_2, t) = \min_{|f| \leq 1} \max_{b = \pm 1} w^\epsilon(x_1 + \epsilon b(1 - f), x_2 - \epsilon b(1 + f), t + \epsilon^2).$$

We expect that $w(x, t) = \lim_{\epsilon \to 0} w^\epsilon$ should solve a PDE.
The PDE is, roughly speaking, the Hamilton-Jacobi-Bellman eqn assoc to our optimal control problem. Sketch of (formal) derivation:

1. Use Taylor expansion to estimate
   \[ w(x_1 + \varepsilon b(1 - f), x_2 - \varepsilon b(1 + f), t + \varepsilon^2). \]

2. Investor chooses \( f \) to make the \( O(\varepsilon) \) terms vanish, since otherwise they kill him; this gives
   \[ f = (\partial_1 w - \partial_2 w)/(\partial_1 w + \partial_2 w). \]

3. The \( O(\varepsilon^2) \) terms are insensitive to \( b = \pm 1 \); they give the nonlinear PDE
   \[ w_t + 2\langle D^2 w \frac{\nabla^\perp w}{\partial_1 w + \partial_2 w}, \frac{\nabla^\perp w}{\partial_1 w + \partial_2 w} \rangle = 0 \quad \text{with} \quad \nabla^\perp w = (-\partial_2 w, \partial_1 w). \]

   This final-value problem is to be solved with \( w = \phi \) at \( t = T \).
More detailed derivation of pde

Dynamic programming principle:

\[ w^\varepsilon(x_1, x_2, t) = \max_{|f| \leq 1} \min_{b = \pm 1} w^\varepsilon(x_1 + \varepsilon b(1 - f), x_2 - \varepsilon b(1 + f), t + \varepsilon^2) \]

Taylor expansion:

\[
w(x_1 + \varepsilon b(1 - f), x_2 - \varepsilon b(1 + f), t + \varepsilon^2) \approx w(x_1, x_2, t) + \varepsilon b(1 - f)w_1 - \varepsilon b(1 + f)w_2 \\
+ \frac{1}{2} w_{11}\varepsilon^2 b^2 (1 - f)^2 - w_{12}\varepsilon^2 b^2 (1 - f)(1 + f) + \frac{1}{2} w_{22}\varepsilon^2 b^2 (1 + f)^2 + w_t\varepsilon^2
\]

After substitution and reorganization:

\[
0 \approx \max_{|f| \leq 1} \min_{b = \pm 1} \{ \varepsilon b[(1 - f)w_1 - (1 + f)w_2] \\
+ \varepsilon^2 b^2 \left[ \frac{1}{2} w_{11}(1 - f)^2 - w_{12}(1 - f)(1 + f) + \frac{1}{2} w_{22}(1 + f)^2 + w_t \right] \}
\]

Order-\(\varepsilon\) term vanishes when

\[ f = \frac{\partial_1 w - \partial_2 w}{\partial_1 w + \partial_2 w}. \]

Note: we expect \(\partial_1 w > 0\) and \(\partial_2 w > 0\). Also: condition \(|f| \leq 1\) is automatic.
Our PDE is geometric. In fact,

$$\partial_t w + 2\langle D^2 w \frac{\nabla \perp w}{\partial_1 w + \partial_2 w}, \frac{\nabla \perp w}{\partial_1 w + \partial_2 w} \rangle = 0$$

can be rewritten as

$$\frac{\partial_t w}{|\nabla w|} = 2\kappa \frac{|\nabla w|^2}{(\partial_1 w + \partial_2 w)^2},$$

where

$$\kappa = -\text{div} \left( \frac{\nabla w}{|\nabla w|} \right)$$

is the curvature of a level set of $w$. Thus the normal velocity of each level set is

$$v_{\text{nor}} = \frac{2\kappa}{(n_1 + n_2)^2}$$

where $\kappa$ is its curvature and $n$ is its unit normal.
Our PDE is the linear heat eqn in disguise. In fact, in the rotated (and scaled) coordinate system

\[ \xi = x_1 - x_2, \quad \eta = x_1 + x_2, \]

each level set of \( w \) is an evolving graph over the \( \xi \) axis. Moreover, the function \( \eta(\xi, t) \) associated with this graph, defined by

\[ w(\xi, \eta(\xi, t), t) = \text{const} \]

solves the linear heat eqn

\[ \eta_t + 2\eta_{\xi\xi} = 0 \quad \text{for } t < T. \]

The proof is elementary: one checks that for the evolving graph, the normal velocity is what our PDE says it should be.

**Corollary**: existence, regularity, and (more or less) explicit solutions for a broad class of final-time data.

Thanks to Y. Giga for this observation.
Main result: If $\phi(x) = w(x, T)$ is smooth, then

$$w(x, t) - C\varepsilon \leq w^\varepsilon(x, t) \leq w(x, t) + C\varepsilon$$

where $C$ is independent of $\varepsilon$. (It grows linearly with $T - t$.)

Method: A verification argument. One inequality is obtained by considering the particular strategy

$$f = (\partial_1 w - \partial_2 w) / (\partial_1 w + \partial_2 w).$$

The other involves showing (as seen in the formal argument) that no other strategy can do better.

For the most standard regret-minimization problem, $\phi(x_1, x_2) = \max\{x_1, x_2\}$ is not smooth. In this case our result is a bit weaker; the errors are of order $\varepsilon|\log \varepsilon|$. 

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Prediction without probability
Goal: show that
\[ w^\varepsilon(x, t) \leq w(x, t) + C\varepsilon. \]

Strategy: Estimate \( w^\varepsilon(z_0, t_0) \) by finding a sequence \((z_1, t_1), (z_2, t_2), \ldots (z_N, t_N)\) such that
- \( t_{j+1} = t_j + \varepsilon^2 \) for each \( j \), and \( t_N = T \).
- \( w^\varepsilon(z_{j+1}, t_{j+1}) \geq w^\varepsilon(z_j, t_j) \) for each \( j \).
- \( w(z_{j+1}, t_{j+1}) = w(z_j, t_j) + O(\varepsilon^3). \)

Since \( N = (T - t_0)/\varepsilon^2 \), it follows easily that
\[ w(z_0, t_0) = w(z_N, t_N) + O(\varepsilon). \]

Since \( w^\varepsilon = w \) at the final time \( T \), we get
\[ w^\varepsilon(z_0, t_0) \leq w^\varepsilon(z_N, t_N) = w(z_N, t_N) \leq w(z_0, t_0) + C\varepsilon. \]
Sketch of one inequality, cont’d

The sequence: Recall the dynamic programming principle

\[ w^\varepsilon(z_0, t_0) = \min_{|f| \leq 1} \max_{b = \pm 1} w^\varepsilon \left( z_0 + \varepsilon b \left( \frac{f-1}{f+1} \right), t_0 + \varepsilon^2 \right) \]

A specific choice of \( f \) gives an inequality; the choice from formal argument gives

\[ \left( \frac{f-1}{f+1} \right) = 2 \frac{\nabla^\perp w}{\partial_1 w + \partial_2 w} \]

evaluated at \((z_0, t_0)\). Call this \( v_0 \). Then

\[ w^\varepsilon(z_0, t_0) \leq \max_{b = \pm 1} w^\varepsilon \left( z_0 + \varepsilon b v_0, t_0 + \varepsilon^2 \right) . \]

Let \( b_0 \) achieve the max, and set \( z_1 = z_0 + \varepsilon b_0 v_0, t_1 = t_0 + \varepsilon^2 \); we have

\[ w^\varepsilon(z_0, t_0) \leq w^\varepsilon(z_1, t_1) . \]

Iterate to find \((z_j, t_j), j = 2, 3, \ldots\)
Proof that \( w(z_{j+1}, t_{j+1}) = w(z_j, t_j) + O(\varepsilon^3) \): use the PDE. (Note: since \( w \) is smooth, Taylor expansion is honest.)

Using the specific choice of \((z_1, t_1)\) we get

\[
w(z_1, t_1) = w(z_0, t_0) + \text{terms of order } \varepsilon \text{ vanish} + \varepsilon^2 \left( \partial_t w + 2\langle D^2 w \frac{\nabla w}{\partial_1 w + \partial_2 w}, \frac{\nabla w}{\partial_1 w + \partial_2 w} \rangle \right) + O(\varepsilon^3)
\]

in which the RHS is evaluated at \((z_0, t_0)\).

Using the PDE for \( w \) this becomes the desired estimate

\[
w(z_1, t_1) = w(z_0, t_0) + \text{terms of order } \varepsilon^2 \text{ vanish} + O(\varepsilon^3).
\]

The argument applies for any \( j \). Error terms come from \( O(\varepsilon^3) \) terms in Taylor expansion; so the implicit constant is uniform if \( D^3 w \) and \( w_{tt} \) are uniformly bounded for all \( x \in \mathbb{R} \) and all \( t < T \).
1. The problem ("prediction with expert advice")
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More realistic experts

So far our experts were very simple (independent of history). Now let’s consider two history-dependent experts.

Keep \(d\) days of history. Typical state is thus \(m = (0001011)_2 \in \{0, 1, \ldots , 2^d - 1\}\). It is updated each day.

Each expert’s prediction is a (known) function of history. The \(q\) expert buys \(f = q(m)\) shares; the \(r\) expert buys \(f = r(m)\) shares.

Otherwise no change: the goal is to optimize the (worst-case) time-\(T\) value of regret wrt best-performing expert, or more generally

\[
\phi(\text{regret wrt } q\ \text{expert}, \text{regret wrt } r\ \text{expert})
\]
Dynamic programming becomes a mess

**Problem:** Dynamic programming doesn’t work so well any more. Apparently

\[ \text{state} = (\text{regret wrt } q \text{ expert, regret wrt } r \text{ expert, history}) \]

so we’re looking for \( 2^d \) distinct functions of space and time, \( w_m(x_1, x_2, t) \). Dynamic programming principle can be formulated (coupling all \( 2^d \) functions). We seem headed for a system of PDEs.

**However:**

(a) Regret accumulates slowly while states change rapidly; so value function should be approx indep of state.

(b) Investor should choose \( f \) to achieve market indifference (at leading order in Taylor expansion).

(c) Accumulation of regret occurs at order \( \epsilon^2 \) (in Taylor expansion).

Using these ideas, we will again get a scalar PDE in the limit \( \epsilon \to 0 \).
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(a) Regret accumulates slowly while states change rapidly; so value function should be approx indep of state.

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Using these ideas, we will again get a scalar PDE in the limit $\varepsilon \to 0$. 

Identifying the PDE

**Formal derivation:** ignore dependence of value function \( w(x_1, x_2, t) \)
on \( \varepsilon \) and \( m \); now

\[
x_1 = \text{regret wrt } q \text{ expert, } x_2 = \text{regret wrt } r \text{ expert.}
\]

If investor chooses \( f \) and market goes up/down (\( b = \pm 1 \)),

\[
x_1 \text{ changes by } b\varepsilon(q(m) - f), \quad x_2 \text{ changes by } b\varepsilon(r(m) - f).
\]

So market indifference at order \( \varepsilon \) requires

\[
w_1(q(m) - f) + w_2(r(m) - f) = -w_1(q(m) - f) - w_2(r(m) - f).
\]

Solve for \( f \): if current state is \( m \), then investor should choose

\[
f = (w_1q(m) + w_2r(m))/(w_1 + w_2).
\]

Accumulation of regret is at order \( \varepsilon^2 \). With \( f \) set by market indifference, change in \( w \) is \( \varepsilon^2 \) times

\[
w_t + \frac{1}{2} (q(m) - r(m))^2 \langle D^2 w, \nabla \nabla^\perp w \rangle.
\]

Worst-case scenario is the one that makes regret accumulate fastest.
Identifying the PDE

Formal derivation: ignore dependence of value function $w(x_1, x_2, t)$ on $\varepsilon$ and $m$; now

$$x_1 = \text{regret wrt q expert}, \ x_2 = \text{regret wrt r expert.}$$

If investor chooses $f$ and market goes up/down ($b = \pm 1$),

$$x_1 \text{ changes by } b\varepsilon(q(m) - f), \ x_2 \text{ changes by } b\varepsilon(r(m) - f).$$

So market indifference at order $\varepsilon$ requires

$$w_1(q(m) - f) + w_2(r(m) - f) = -w_1(q(m) - f) - w_2(r(m) - f).$$

Solve for $f$: if current state is $m$, then investor should choose

$$f = (w_1 q(m) + w_2 r(m))/(w_1 + w_2).$$

Accumulation of regret is at order $\varepsilon^2$. With $f$ set by market indifference, change in $w$ is $\varepsilon^2$ times

$$w_t + \frac{1}{2} (q(m) - r(m))^2 \left\langle D^2 w \frac{\nabla^\perp w}{\partial_1 w + \partial_2 w}, \frac{\nabla^\perp w}{\partial_1 w + \partial_2 w} \right\rangle.$$

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\]

Worst-case scenario is the one that makes regret accumulate fastest.
Recall: accumulation of regret per step at state $m$ is

$$\frac{1}{2} (q(m) - r(m))^2 \langle D^2 w \frac{\nabla \perp w}{\partial_1 w + \partial_2 w}, \frac{\nabla \perp w}{\partial_1 w + \partial_2 w} \rangle.$$ 

Essentially a problem from graph theory: seek

$$\lim_{N \to \infty} \max_{\text{paths of length } N} \frac{1}{N} \sum_{j=1}^{N} (q(m_j) - r(m_j))^2.$$ 

In fact:

- It suffices to consider cycles.
- There are good algorithms for finding optimal cycles.
Identifying the PDE, cont’d

Thus finally: the PDE is

\[
wt + \frac{1}{2} C_* \left\langle D^2 w \frac{\nabla \perp w}{\partial_1 w + \partial_2 w}, \frac{\nabla \perp w}{\partial_1 w + \partial_2 w} \right\rangle = 0,
\]

where

\[
C_* = \max_{\text{cycles}} \frac{1}{\text{cycle length}} \sum (q(m_j) - r(m_j))^2.
\]

Summarizing: for two history-dependent experts,

- Investor’s choice of \( f \) depends on the state as well as on \( \nabla w(x) \); it achieves leading-order market indifference.

- The value function \( w \) solves (almost) the same eqn as before (still reducible to the linear heat eqn!). All that changes is the “diffusion coefficient.”

- Rigorous analysis still uses a verification argument (though there are some new subtleties).
Can something similar be done for many history-dependent experts?

- If there are $K$ experts then $w = w(x_1, \cdots, x_K, t)$.
- Market indifference at order $\varepsilon$ still gives a formula for $f$.
- Accumulation of regret sees $D^2 w$ and $Dw$ (not just a scalar quantity built from them); so the graph problem depends nontrivially on $D^2 w$ and $Dw$.
- The formal PDE is much more nonlinear than for two experts. (Analysis: in progress.)
Mathematical messages

- Stock prediction problem has a continuous-time limit. Reduction to linear heat eqn provides a rather explicit solution.

- It provides another example where a deterministic two-person game leads to 2nd order nonlinear PDE. (For earlier examples, see Kohn-Serfaty CPAM 2006 and CPAM 2010.)

- Our analysis was elementary, since PDE is linked to linear heat eqn. In other settings, when PDE solution is not smooth, convergence has been proved (without a rate) using viscosity methods.
Stepping back

Comparison to the machine learning literature

- ML is mostly discrete. It was known that for the unscaled game, worst-case regret after $N$ steps is of order $\sqrt{N}$ (compare: our parabolic scaling). Our analysis gives the prefactor.

- ML guys are smart. For the classic problem of minimizing worst-case regret, Andoni & Panigrahy found the same strategies that come from our analysis (arXiv:1305.1359) – but didn’t have the tools to prove they’re optimal.

- The link to a linear heat eqn gives surprisingly explicit solutions in the continuum limit.
Stepping back

Is this just a curiosity?

Key point: since behavior over many time steps is of interest, continuous time viewpoint should be useful.

But: the stock prediction problem is very simple: a binary time series and a linear “loss function.” What about other examples?

One might ask: when is worst-case regret minimization a good idea? Not obvious...
Happy Birthday, Yoshi!