Estimates for the Heat Kernel on Weighted Graphs

A Presentation of Some Recent Developments.

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by

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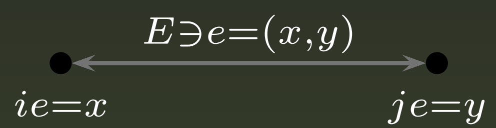

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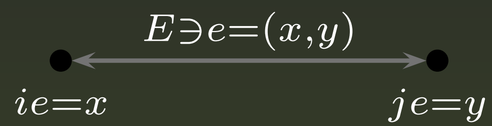

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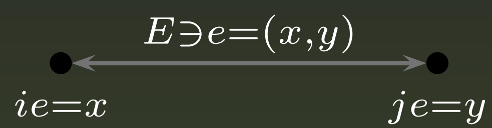

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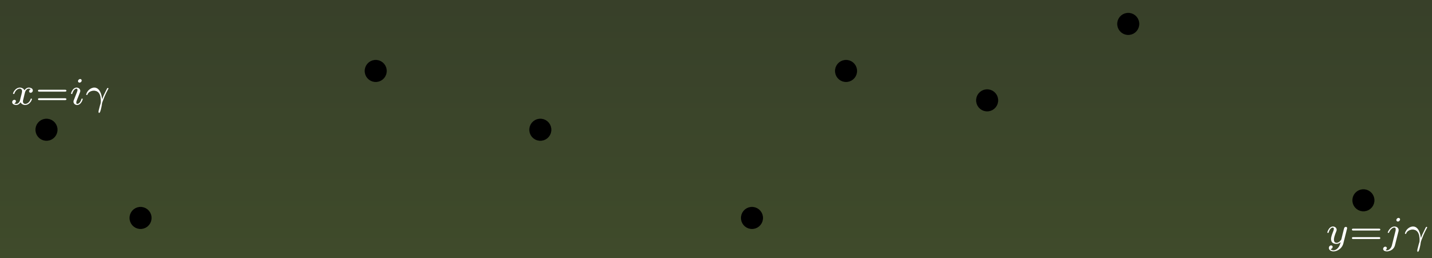

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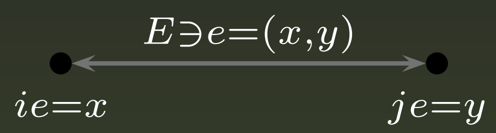

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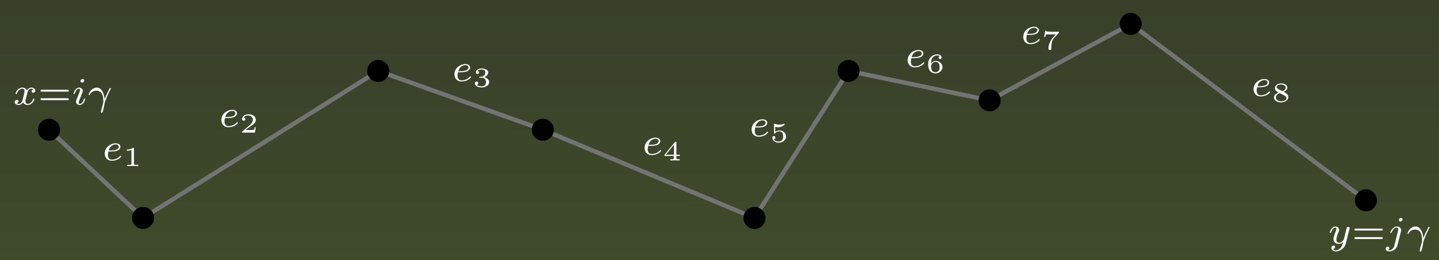

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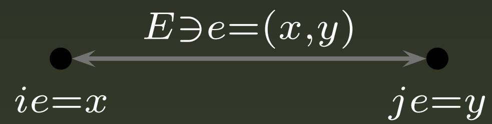

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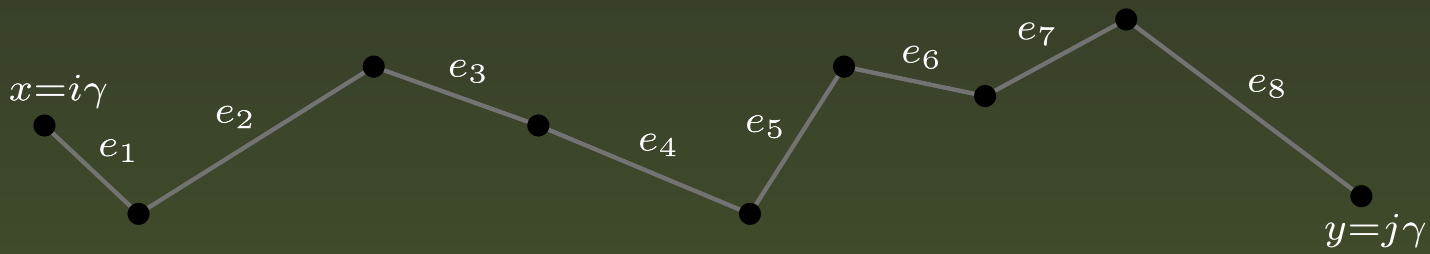

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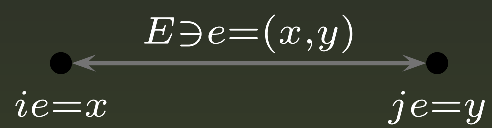

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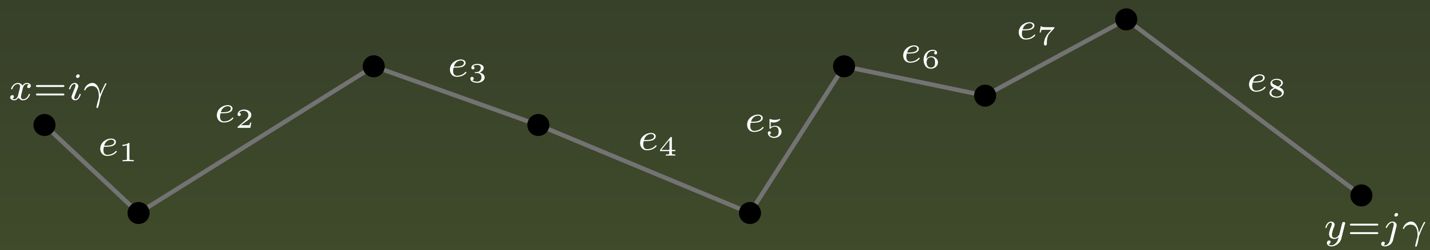

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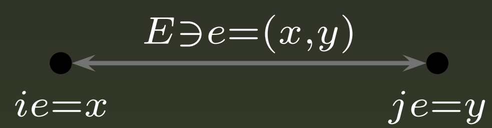

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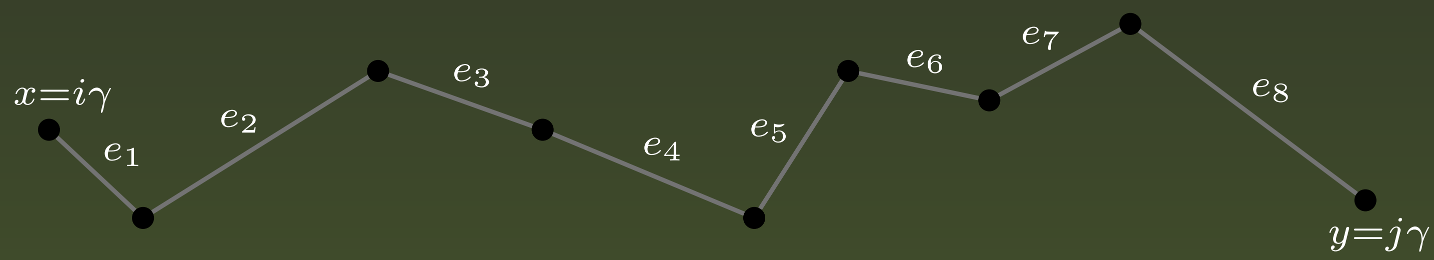

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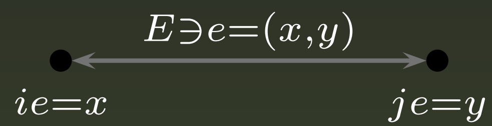

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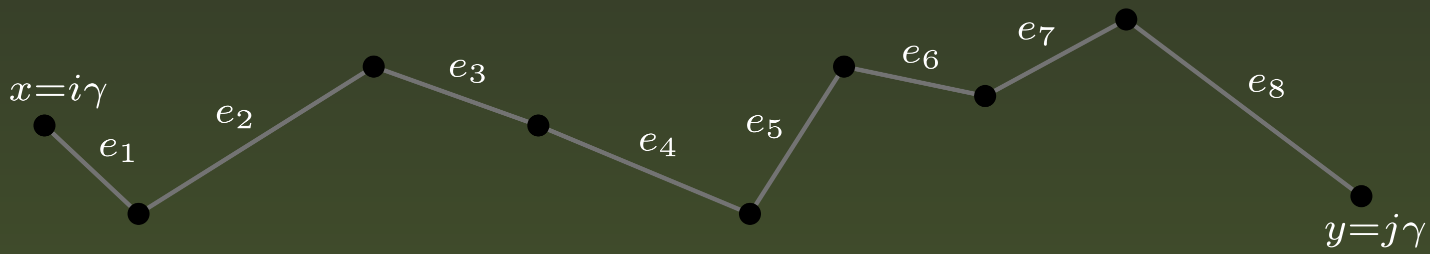

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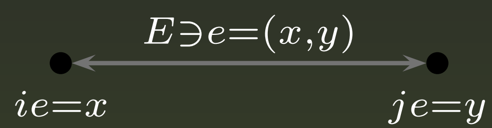

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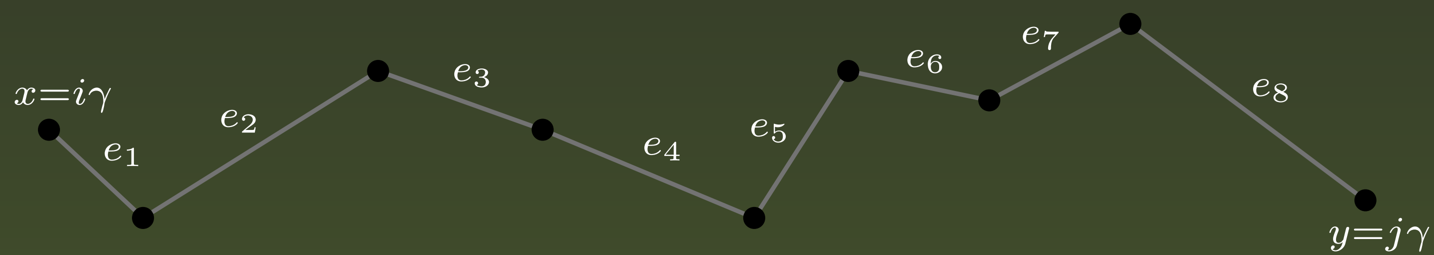

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Weights : A mapping $b \colon E \longrightarrow (0, \infty)$. We assume that X is **symmetric**, that is,

$$e = (x,y) \in E \Longrightarrow \overline{e} = (y,x) \in E \quad \text{and} \quad b(\overline{e}) = b(e).$$

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The discrete Laplacian on X is the operator $\Delta\colon l^2(X) \longrightarrow l^2(X)$ defined by

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where $\delta_x \in l^2(X)$ is the unit mass concentrated at the site $x\in X$. The function $p_t(x,y)$ is called the **heat kernel** on X. The Markov chain $(X_t \mid t\geq 0)$ 'jumps' from site x to a neighbouring site y with probability

$$\frac{b\big((x,y)\big)}{\sum\limits_{\substack{e\in E,\\ ie=x}} b(e)}.$$

That means, the weight b measures the 'conductance' of edges.

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$$\frac{\mathrm{e}^{-b_{\max} M t}}{\sqrt{2\pi}} \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{t b(e)}{|\gamma|} \right)$$

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Combinatorial term: Upper bound for the probability for jumping along γ.

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Stochastic term from the dynamics of the Markov process.

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This gives a probability for making a way of length $d_0(x,y)$ in time t:

$$\left(\frac{M b_{\max} t}{d_0(x,y)}\right)^{d_0(x,y)}.$$

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Now, $(tb_{\min}/x)^x$ is maximal at $x = tb_{\min}/\mathrm{e}$ and for $k \geq d_0(x,y) > tb_{\min}/\mathrm{e}$ it is monotonuously decreasing with supremum at $k = d_0(x,y)$.

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Inserting into the lower estimate one obtains

$$p_t(x,y) \geq \frac{\mathrm{e}^{-b_{\max}Mt}}{\sqrt{2\pi}} \sup_{\gamma\in\Gamma(x,y)} \left(\frac{tb_{\min}}{|\gamma|}\right)^{|\gamma|} = \frac{\mathrm{e}^{-b_{\max}Mt}}{\sqrt{2\pi}} \sup_{k\geq d_0(x,y)} \left(\frac{tb_{\min}}{k}\right)^{k}.$$

Now, $(tb_{\min}/x)^x$ is maximal at $x = tb_{\min}/\mathrm{e}$ and for $k \geq d_0(x,y) > tb_{\min}/\mathrm{e}$ it is monotonuously decreasing with supremum at $k = d_0(x,y)$. This yields the two cases:

$$p_t(x,y) \geq \begin{cases} (1-E)\cdot \dfrac{\mathrm{e}^{t(b_{\min}/\mathrm{e}-b_{\max}M)}}{\sqrt{2\pi}}, & \text{if } d_0(x,y) \leq tb_{\min}/\mathrm{e}; \\[2ex] \dfrac{\mathrm{e}^{-b_{\max}Mt}}{\sqrt{2\pi}} \left(\dfrac{tb_{\min}}{d_0(x,y)}\right)^{d_0(x,y)}, & \text{otherwise.} \end{cases}$$

Where the cut-off error $E \geq 0$ depends on $t/b_{\min}$.

A Physical Interpretation of the Estimates

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The estimates represent a balance between **diffusion** and **conductance**:

$$\frac{e^{-b_{\max}Mt}}{\sqrt{2\pi}} \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{tb(e)}{|\gamma|} \right)$$

$$\leq$$

$$p_t(x,y)$$

$$\leq$$

$$e^{b_{\max}Mt+1} \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{b(e)}{b_{\max}} \right) \left(\frac{eMb_{\max}t}{d_0(x,y)} \right)^{d_0(x,y)} .$$

A Physical Interpretation of the Estimates

The estimates represent a balance between **diffusion** and **conductance**:

$$\frac{\mathrm{e}^{-b_{\max} M t}}{\sqrt{2\pi}} \sup_{\gamma \in \Gamma(x,y)} \left(\prod_{e \in \gamma} \frac{t b(e)}{|\gamma|} \right)$$

$$\leq$$

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$$\mathrm{e}^{b_{\max} M t + 1} \sup_{\gamma \in \Gamma(x,y)} \left(\prod_{e \in \gamma} \frac{b(e)}{b_{\max}} \right) \left(\frac{\mathrm{e} M b_{\max} t}{d_0(x,y)} \right)^{d_0(x,y)} .$$

But a **diffusive** term is missing in the upper estimate.

Derivation of the Upper Estimate: Basic Principles

Derivation of the Upper Estimate: Basic Principles

We represent the heat kernel as

$$p_t(x, y) = \lim_{n \to \infty} \left[\left(I + \frac{t}{n} \Delta \right)^n \delta_x \right] (y).$$

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Define operators on $l^2(X)$ by

$$Sf(x) \stackrel{\text{def}}{=} \sum_{ie=x} b(e) f(je), \text{ that is, the ‘off-diagonal’ part of } \Delta, \text{ and}$$

$$D \stackrel{\text{def}}{=} \left(-\sum_{ie=x} b(e) \right) \mathbb{I}, \quad D_{\min} \stackrel{\text{def}}{=} -N b_{\min} \mathbb{I}, \quad D_{\max} \stackrel{\text{def}}{=} -M b_{\max} \mathbb{I}.$$

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Then $\Delta = D + S$, and the estimates $D_{\max} \le D \le D_{\min} \le 0$ entail by induction:

Lemma: For $f \in l^2(X)$, $f \ge 0$, $n \in \mathbb{N}$, and $s > 0$ small enough holds

$$0 \le \big(\mathbb{I} + s(D_{\max} + S)\big)^n f \ \le \quad (\mathbb{I} + s\Delta)^n f \quad \le \ \big(\mathbb{I} + s(D_{\min} + S)\big)^n f.$$

Derivation of the Upper Estimate: Calculation

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I} + \frac{t}{n}\Delta\right)^n \delta_x\right](y) \leq \left[\left(\mathbb{I} - \frac{tNb_{\min}}{n}\mathbb{I} + \frac{t}{n}S\right)^n \delta_x\right](y)$$

This is the basic estimate for the n-th order approximation of $p_t(x, y)$ that follows from the upper bound in the Lemma.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I} + \frac{t}{n}\Delta\right)^n \delta_x\right](y) \leq \left[\left(\mathbb{I} - \frac{tNb_{\min}}{n}\mathbb{I} + \frac{t}{n}S\right)^n \delta_x\right](y)$$

$$= \sum_{k=0}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \cdot \left[\left(\frac{t}{n}S\right)^k \delta_x\right](y)$$

Evaluation of the binomial yields this expression.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I} + \frac{t}{n}\Delta\right)^n \delta_x\right](y) \leq \left[\left(\mathbb{I} - \frac{tNb_{\min}}{n}\mathbb{I} + \frac{t}{n}S\right)^n \delta_x\right](y)$$

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Set $b(\gamma) \stackrel{\text{def}}{=} \prod_{e\in\gamma} b(e)$.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I}+\frac{t}{n}\Delta\right)^n\delta_x\right](y) \le \left[\left(\mathbb{I}-\frac{tNb_{\min}}{n}\mathbb{I}+\frac{t}{n}S\right)^n\delta_x\right](y)$$

$$=\sum_{k=0}^{n}\binom{n}{k}\left(1-\frac{tNb_{\min}}{n}\right)^{n-k}\cdot\left[\left(\frac{t}{n}S\right)^k\delta_x\right](y)$$

Set $b(\gamma) \stackrel{\text{def}}{=} \prod_{e\in\gamma} b(e)$. Then $S^k\delta_x = \sum_{\substack{i\gamma=x,\\ |\gamma|=k}} b(\gamma)\delta_{j\gamma}$.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I}+\frac{t}{n}\Delta\right)^{n}\delta_x\right](y) \le \left[\left(\mathbb{I}-\frac{tNb_{\min}}{n}\mathbb{I}+\frac{t}{n}S\right)^{n}\delta_x\right](y)$$

$$=\sum_{k=0}^{n}\binom{n}{k}\left(1-\frac{tNb_{\min}}{n}\right)^{n-k}\cdot\left[\left(\frac{t}{n}S\right)^{k}\delta_x\right](y)$$

Set $b(\gamma)\stackrel{\text{def}}{=}\prod_{e\in\gamma} b(e)$. Then $S^k\delta_x=\sum_{\substack{i\gamma=x,\\|\gamma|=k}} b(\gamma)\delta_{j\gamma}$. Thus $\left(S^k\delta_x\right)(y)=\sum_{\substack{\gamma\in\Gamma(x,y),\\|\gamma|=k}} b(\gamma)$.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I}+\frac{t}{n}\Delta\right)^n \delta_x\right](y) \leq \left[\left(\mathbb{I}-\frac{tNb_{\min}}{n}\mathbb{I}+\frac{t}{n}S\right)^n \delta_x\right](y)$$

$$= \sum_{k=0}^{n} \binom{n}{k} \left(1-\frac{tNb_{\min}}{n}\right)^{n-k} \cdot \left(\frac{t}{n}\right)^k \sum_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} b(\gamma).$$

Set $b(\gamma) \stackrel{\text{def}}{=} \prod_{e\in\gamma} b(e)$. Then $S^k\delta_x = \sum_{\substack{i\gamma=x,\\ |\gamma|=k}} b(\gamma)\delta_{j\gamma}$. Thus $\left(S^k\delta_x\right)(y) = \sum_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} b(\gamma)$.

Inserting in the last term, we obtain this.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I}+\frac{t}{n}\Delta\right)^{n}\delta_x\right](y)\leq\left[\left(\mathbb{I}-\frac{tNb_{\min}}{n}\mathbb{I}+\frac{t}{n}S\right)^{n}\delta_x\right](y)$$

$$=\sum_{k=d_0(x,y)}^{n}\binom{n}{k}\left(1-\frac{tNb_{\min}}{n}\right)^{n-k}\cdot\left(\frac{t}{n}\right)^{k}\sum_{\substack{\gamma\in\Gamma(x,y),\\|\gamma|=k}}b(\gamma).$$

Only terms with $k\geq d_0(x,y)$ contribute to the sum.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I}+\frac{t}{n}\Delta\right)^n \delta_x\right](y) \le \left[\left(\mathbb{I}-\frac{tNb_{\min}}{n}\mathbb{I}+\frac{t}{n}S\right)^n \delta_x\right](y)$$

$$= \sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1-\frac{tNb_{\min}}{n}\right)^{n-k} \cdot \left(\frac{t}{n}\right)^k \sum_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} b(\gamma).$$

Now $\#\{\gamma \in \Gamma(x,y) \mid |\gamma| = k\} \le M^k$.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I} + \frac{t}{n}\Delta\right)^n \delta_x\right](y) \leq \left[\left(\mathbb{I} - \frac{tNb_{\min}}{n}\mathbb{I} + \frac{t}{n}S\right)^n \delta_x\right](y)$$

$$\leq \sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \cdot \left(\frac{t}{n}\right)^k \underbrace{M^k \sup_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} b(\gamma)}.$$

Now $\#\{\gamma \in \Gamma(x,y) \mid |\gamma| = k\} \leq M^k$.
Therefore we can estimate the last term by this from above.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I}+\frac{t}{n}\Delta\right)^{n}\delta_x\right](y) \le \left[\left(\mathbb{I}-\frac{tNb_{\min}}{n}\mathbb{I}+\frac{t}{n}S\right)^{n}\delta_x\right](y)$$

$$\le \sum_{k=d_0(x,y)}^{n}\binom{n}{k}\left(1-\frac{tNb_{\min}}{n}\right)^{n-k}\cdot\left(\frac{t}{n}\right)^{k}M^{k}\sup_{\substack{\gamma\in\Gamma(x,y),\\|\gamma|=k}}\left(\prod_{e\in\gamma}b(e)\right).$$

Re-inserting $b(\gamma)=\prod_{e\in\gamma}b(e)$ we get this.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I}+\frac{t}{n}\Delta\right)^n\delta_x\right](y) \leq \left[\left(\mathbb{I}-\frac{tNb_{\min}}{n}\mathbb{I}+\frac{t}{n}S\right)^n\delta_x\right](y)$$

$$\leq \sum_{k=d_0(x,y)}^{n}\binom{n}{k}\left(1-\frac{tNb_{\min}}{n}\right)^{n-k}\cdot\underbrace{\left(\frac{tMb_{\max}}{n}\right)^k \sup_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}}\left(\prod_{e\in\gamma}\frac{b(e)}{b_{\max}}\right)}.$$

Dividing and multiplying by $b_{\max}$ yields this.

Derivation of the Upper Estimate: Calculation

$$\left[\left(\mathbb{I}+\frac{t}{n}\Delta\right)^n \delta_x\right](y) \leq \left[\left(\mathbb{I}-\frac{tNb_{\min}}{n}\mathbb{I}+\frac{t}{n}S\right)^n \delta_x\right](y)$$

$$\leq \sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1-\frac{tNb_{\min}}{n}\right)^{n-k} \cdot \left(\frac{tMb_{\max}}{n}\right)^k \sup_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} \left(\prod_{e\in\gamma}\frac{b(e)}{b_{\max}}\right)$$

$$\leq \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma}\frac{b(e)}{b_{\max}}\right) \cdot \sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1-\frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^k .$$

Estimating $\sup_{\substack{\gamma\in\Gamma(x,y),\\ |\gamma|=k}} \ldots \leq \sup_{\gamma\in\Gamma(x,y)} \ldots$, we pull the supremum out of the sum.

Stirling's Formula and the Limit $n \to \infty$

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$$\sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}.$$

The sum is the only part that depends on n. So we consider it separately.

Stirling's Formula and the Limit $n \to \infty$

$$\sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}$$

$$= \sum_{k=m}^{n} \binom{n}{k} \left(1 - \frac{d}{n}\right)^{n-k} \left(\frac{c}{n}\right)^{k}.$$

Substituting $c \stackrel{\text{def}}{=} tMb_{\max}$, $d \stackrel{\text{def}}{=} tNb_{\min}$, and $m \stackrel{\text{def}}{=} d_0(x,y)$, reveals the general structure.

Stirling's Formula and the Limit $n \to \infty$

$$\sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}$$

$$= \left(1 - \frac{d}{n}\right)^{n} \sum_{k=m}^{n} \binom{n}{k} \left(\frac{c}{n-d}\right)^{k}.$$

$$c \overset{\text{def}}{=} tMb_{\max},\ d \overset{\text{def}}{=} tNb_{\min},\ m \overset{\text{def}}{=} d_0(x,y)$$

We pull this factor out of the sum.

Stirling's Formula and the Limit $n \to \infty$

$$\sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}$$

$$= \left(1 - \frac{d}{n}\right)^{n} \sum_{k=m}^{n} \binom{n}{k} \left(\frac{c}{n-d}\right)^{k} = \left(1 - \frac{d}{n}\right)^{n} \sum_{k=m}^{n} \binom{n}{k} \left(\frac{c'}{n}\right)^{k}.$$

$$c \stackrel{\text{def}}{=} tMb_{\max},\ d \stackrel{\text{def}}{=} tNb_{\min},\ m \stackrel{\text{def}}{=} d_0(x,y),\ c' \stackrel{\text{def}}{=} \frac{c}{1-d/n}.$$

Substituting $c' \stackrel{\text{def}}{=} c/(1-d/n)$ simplifys the summands.

Stirling's Formula and the Limit $n \to \infty$

$$\sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}$$

$$= \left(1 - \frac{d}{n}\right)^{n} \sum_{k=m}^{n} \binom{n}{k} \left(\frac{c}{n-d}\right)^{k} = \left(1 - \frac{d}{n}\right)^{n} \sum_{k=m}^{n} \binom{n}{k} \left(\frac{c'}{n}\right)^{k}.$$

$$\leq \left(1 - \frac{d}{n}\right)^{n} \left(\frac{c'}{m}\right)^{m} \left(1 + \frac{m}{n-m}\right)^{n-m} \mathrm{e} \sqrt{1 + \frac{m}{n-m}}\, \mathrm{e}^{\frac{1}{12(n-1)}} \left(1 + \frac{c'}{n}\right)^{n-m}.$$

$$c \overset{\text{def}}{=} tMb_{\max},\ d \overset{\text{def}}{=} tNb_{\min},\ m \overset{\text{def}}{=} d_0(x,y),\ c' \overset{\text{def}}{=} \frac{c}{1 - d/n}.$$

An estimate based on Stirling's formula $\Gamma(z) = z^z \mathrm{e}^{-z} \mathrm{e}^{\vartheta/(12z)} \sqrt{2\pi/z}$, with $\vartheta \in (0, 1)$, allows us to estimate the sum as shown. See [MS00, Lemma 3(b)] for details.

Stirling's Formula and the Limit $n \to \infty$

$$\sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}$$

$$\leq \left(1 - \frac{d}{n}\right)^{n} \left(\frac{cn}{m(n-d)}\right)^{m} \left(1 + \frac{m}{n-m}\right)^{n-m} \mathrm{e} \sqrt{1 + \frac{m}{n-m}}\, \mathrm{e}^{\frac{1}{12(n-1)}} \left(1 + \frac{c}{n-d}\right)^{n-m}.$$

$$c \stackrel{\text{def}}{=} tMb_{\max},\ d \stackrel{\text{def}}{=} tNb_{\min},\ m \stackrel{\text{def}}{=} d_0(x,y)$$

We resubstitute c'.

Stirling's Formula and the Limit $n \to \infty$

$$\lim_{n\to\infty} \sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}$$

$$\leq \quad e^{-d} \quad \cdot \quad \left(\frac{c}{m}\right)^{m} \quad \cdot \quad e^{m} \quad \cdot \quad e \quad \cdot \quad 1 \quad \cdot \quad e^{c}.$$

$$\left(1 - \frac{d}{n}\right)^{n} \left(\frac{cn}{m(n-d)}\right)^{m} \left(1 + \frac{m}{n-m}\right)^{n-m} e \sqrt{1 + \frac{m}{n-m}}\; e^{\frac{1}{12(n-1)}} \left(1 + \frac{c}{n-d}\right)^{n-m}.$$

$$c \overset{\text{def}}{=} tMb_{\max},\; d \overset{\text{def}}{=} tNb_{\min},\; m \overset{\text{def}}{=} d_0(x,y)$$

Now, we have to take the limit $n \to \infty$.

Stirling's Formula and the Limit $n \to \infty$

$$\lim_{n\to\infty} \sum_{k=d_0(x,y)}^{n} \binom{n}{k} \left(1 - \frac{tNb_{\min}}{n}\right)^{n-k} \left(\frac{tMb_{\max}}{n}\right)^{k}$$

$$\leq \quad \mathrm{e}^{-d} \quad \cdot \quad \left(\frac{c}{m}\right)^{m} \quad \cdot \quad \mathrm{e}^{m} \quad \cdot \quad \mathrm{e} \quad \cdot \quad 1 \quad \cdot \quad \mathrm{e}^{c}.$$

$$= \quad \mathrm{e}^{-tNb_{\min}} \left(\frac{\mathrm{e}tMb_{\max}}{d_0(x,y)}\right)^{d_0(x,y)} \mathrm{e}^{tMb_{\max}+1}.$$

$$c \stackrel{\text{def}}{=} tMb_{\max},\ d \stackrel{\text{def}}{=} tNb_{\min},\ m \stackrel{\text{def}}{=} d_0(x,y)$$

Finally, we re-insert the definitions of c, d, and m.

The New Upper Estimate

The New Upper Estimate

Collecting the results we obtain

$$p_t(x,y) \le \quad \mathrm{e}^{-tNb_{\min}} \quad \mathrm{e}^{tMb_{\max}+1} \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{b(e)}{b_{\max}} \right) \left(\frac{\mathrm{e}tMb_{\max}}{d_0(x,y)} \right)^{d_0(x,y)} .$$

The New Upper Estimate

Collecting the results we obtain

$$p_t(x,y) \le \mathrm{e}^{-tNb_{\min}} \mathrm{e}^{tMb_{\max}+1} \sup_{\gamma\in\Gamma(x,y)} \left(\prod_{e\in\gamma} \frac{b(e)}{b_{\max}} \right) \left(\frac{\mathrm{e}tMb_{\max}}{d_0(x,y)} \right)^{d_0(x,y)} .$$

The **diffusive term** $\mathrm{e}^{-tNb_{\min}}$ tends to 1 for $b_{\min} \longrightarrow 0$, reproducing the upper estimate of [MS00] in this case. Thus we obtained a proper generalization.